

# **Intramolecular Monomer-on-Monomer (MoM) Mitsunobu Cyclization for the Synthesis of Benzo-fused Thiadiazepine-dioxides<sup>i</sup>**

Pradip K. Maity, Quirin M. Kainz, Saquib Faisal, Alan Rolfe, Thiwanka B. Samarakoon, Fatima Z. Basha, Oliver Reiser, and Paul R. Hanson\*

## **Supporting Information**

### **1. NMR spectra**

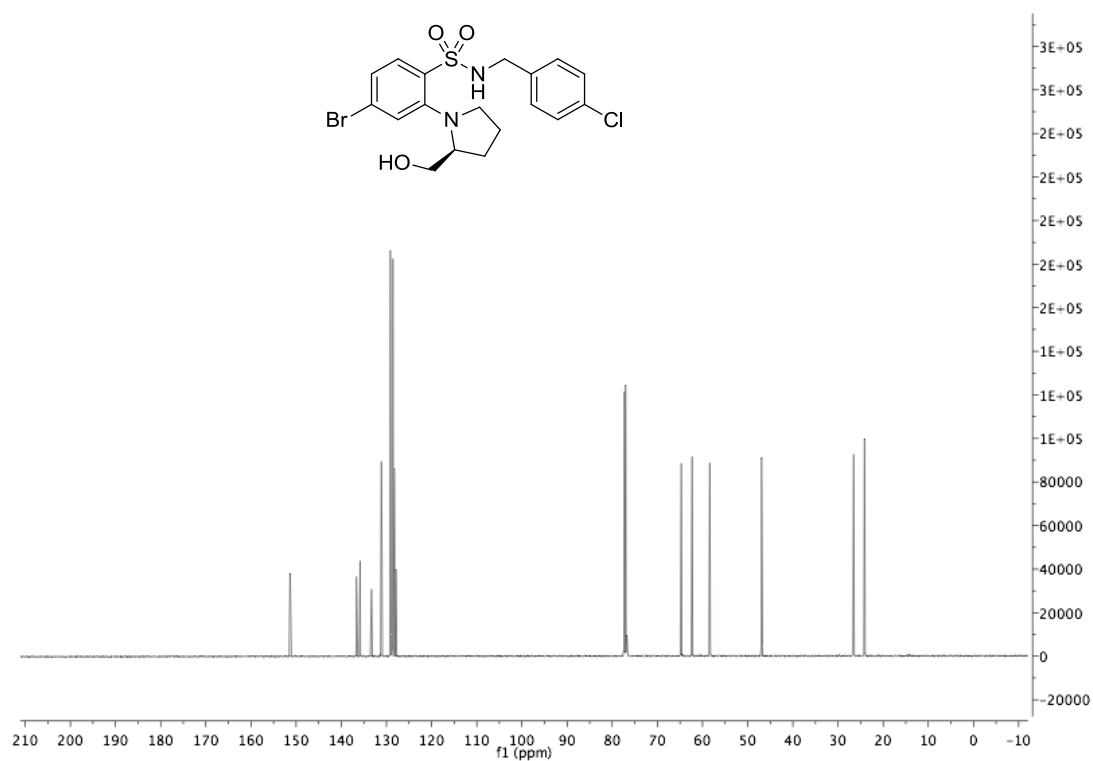
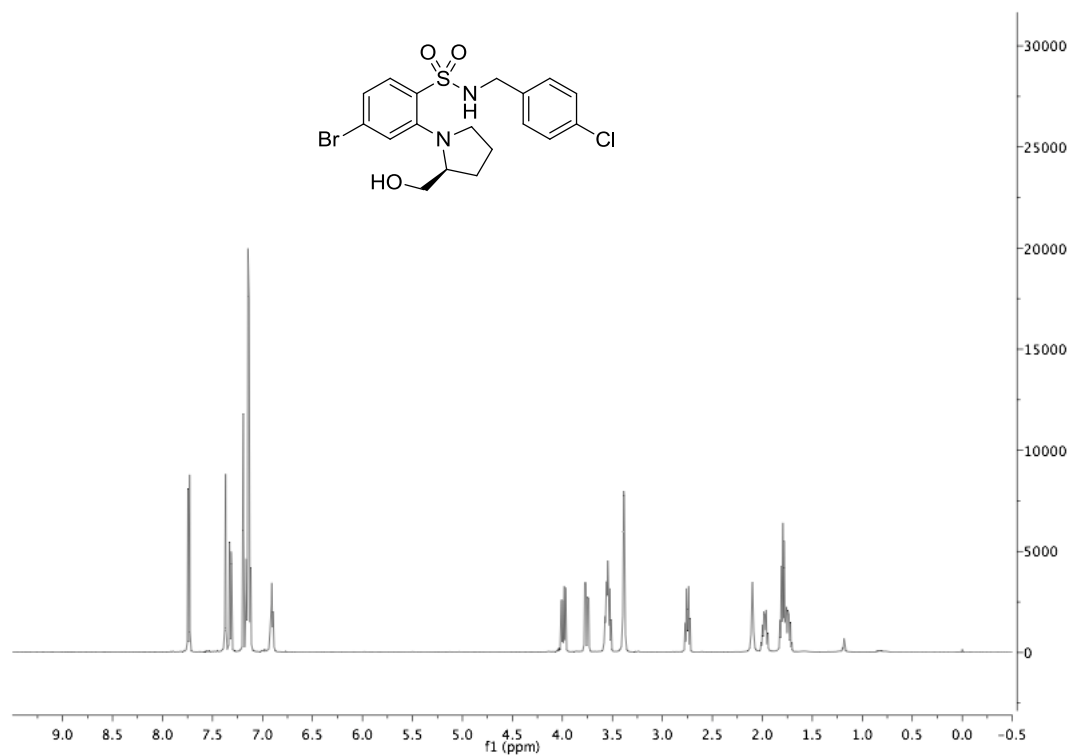
**S2**

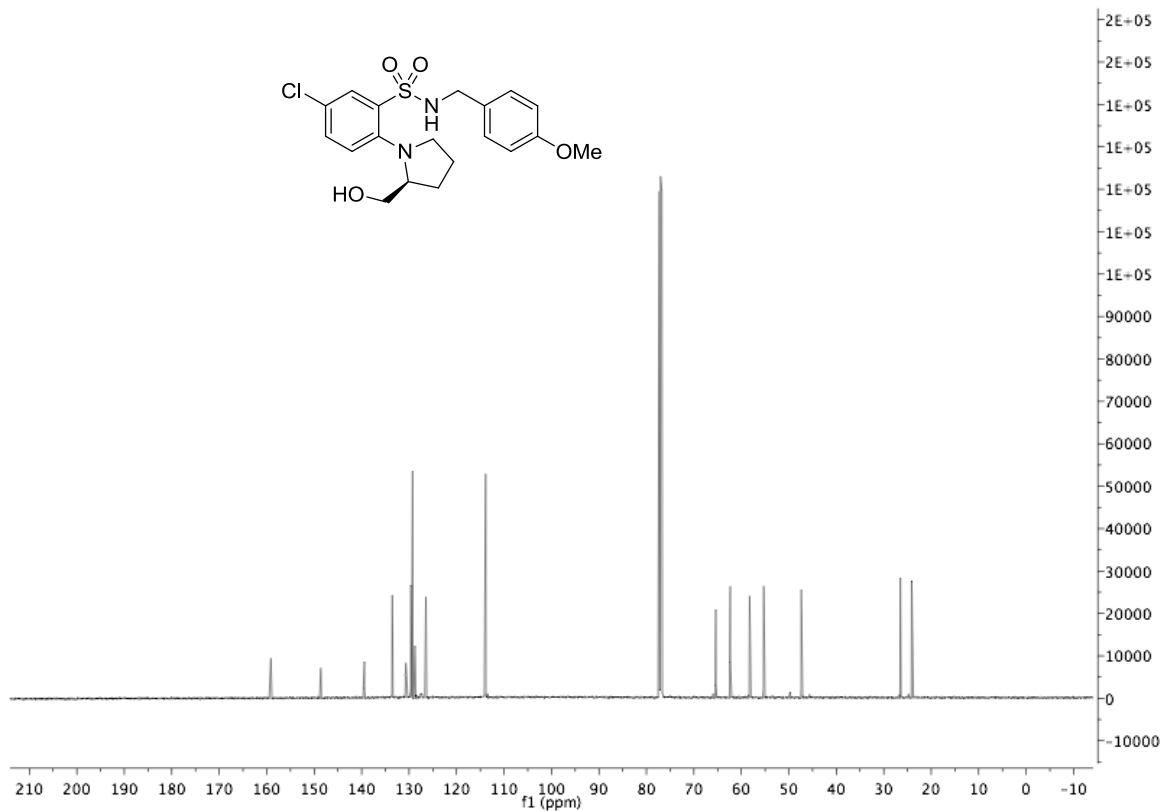
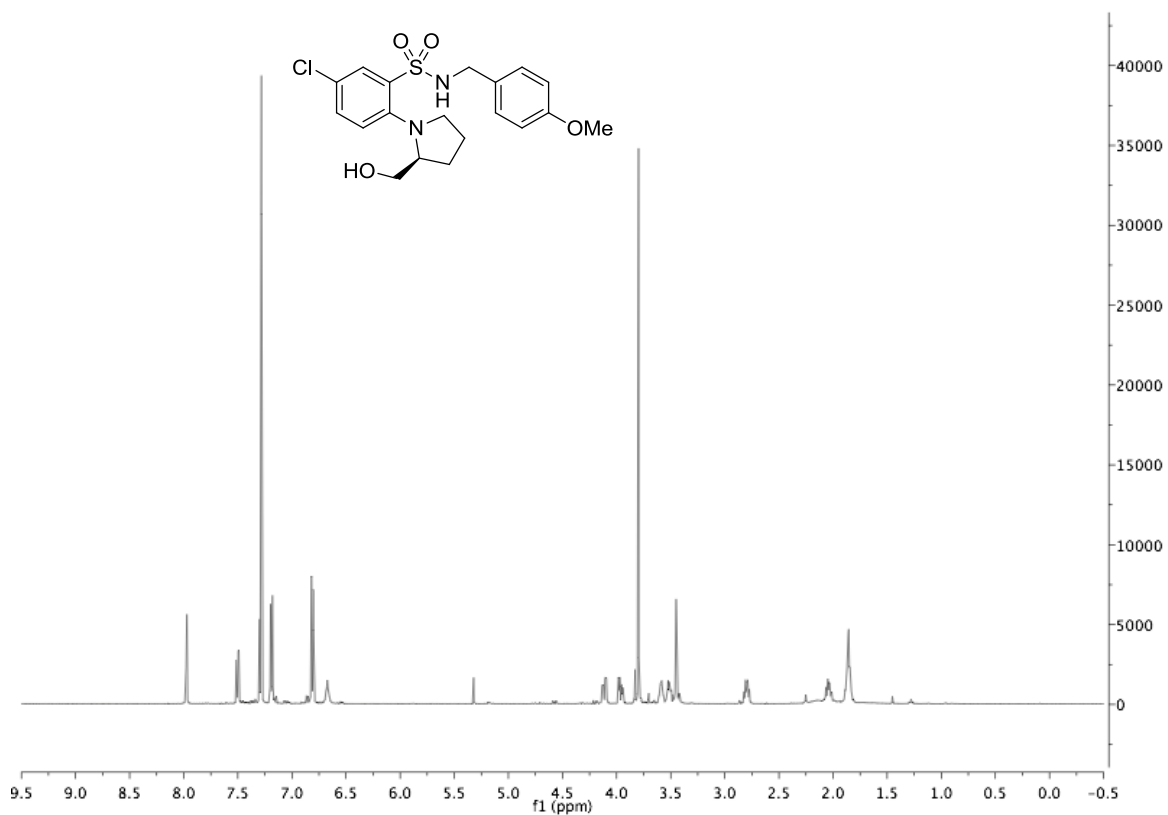
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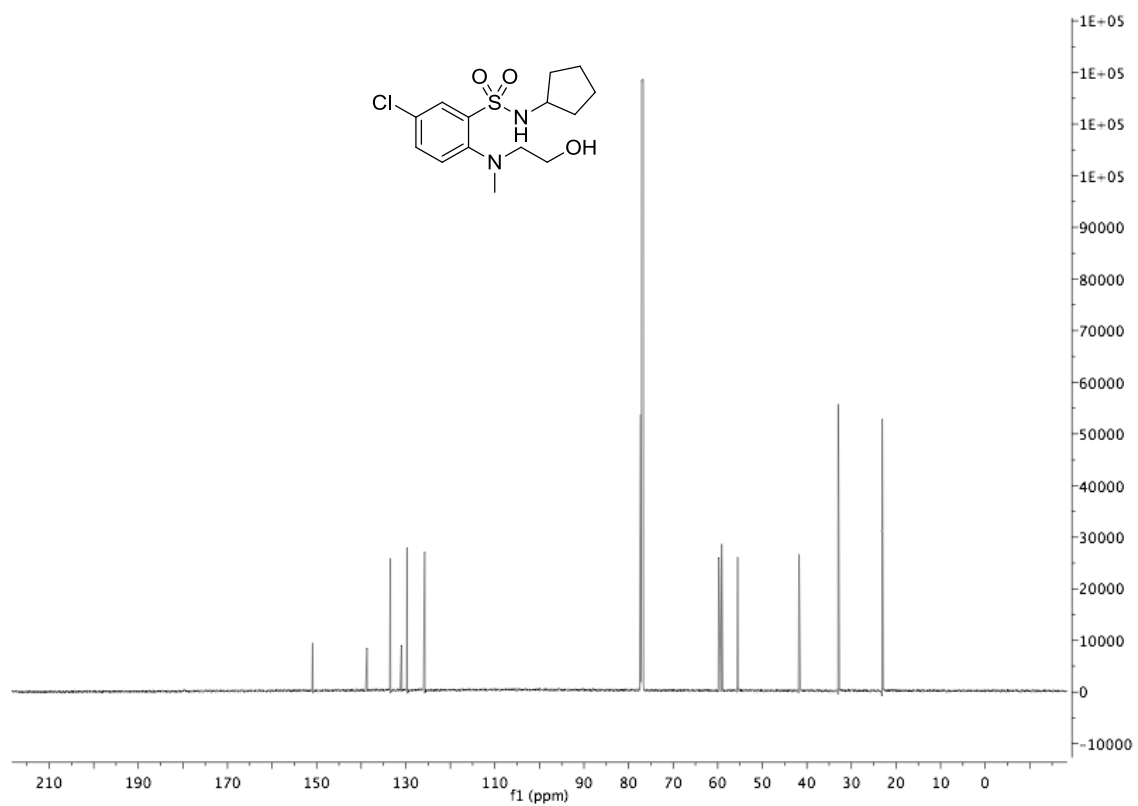
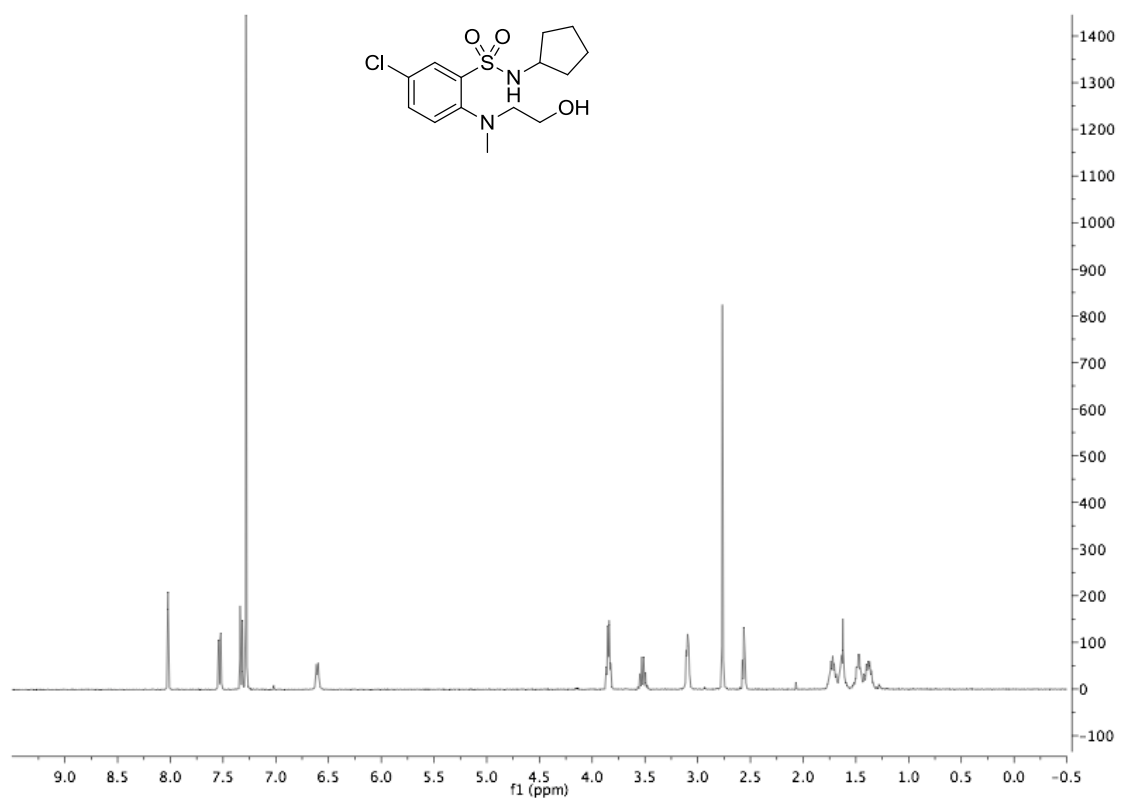
<sup>i</sup> Reproduced with permission from: P. K. Maity, Q. M. Kainz, S. Faisal, A. Rolfe, T. B. Samarakoon, F. Z. Basha, O. Reiser, P. R. Hanson, *Chem. Commun.* **2011**, 47, 12524-12526. Copyright 2011 The Royal Society of Chemistry.

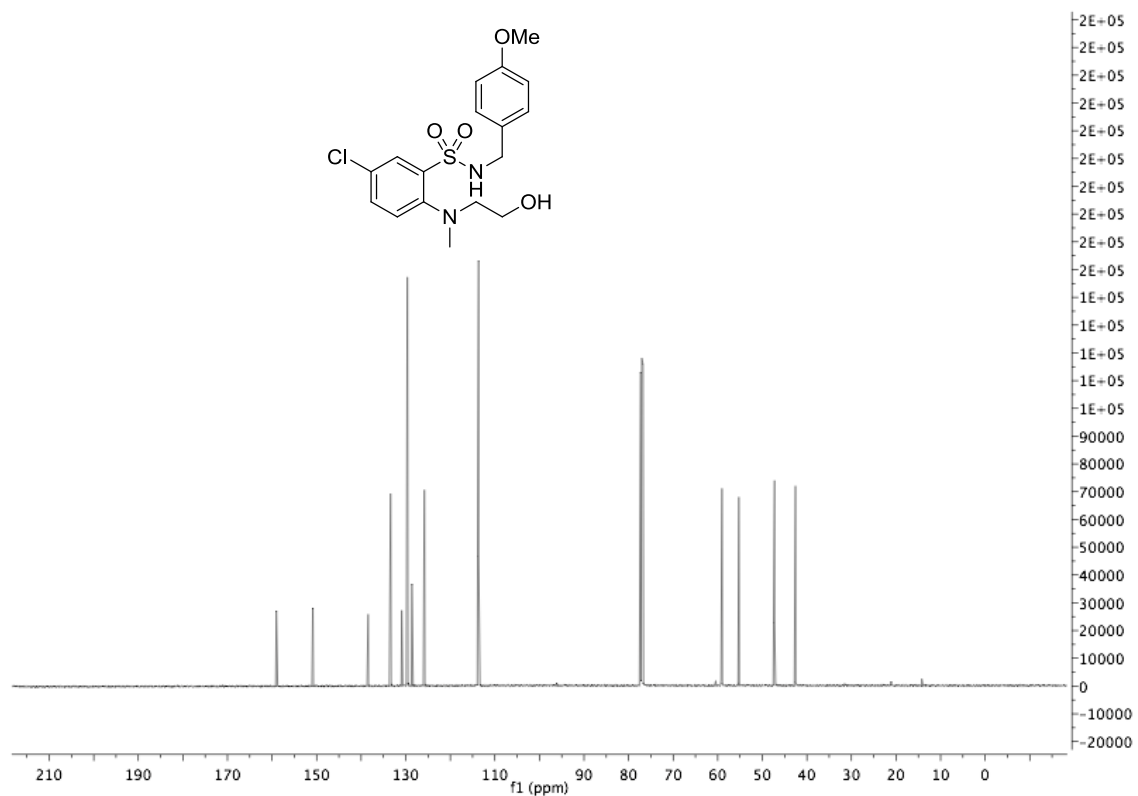
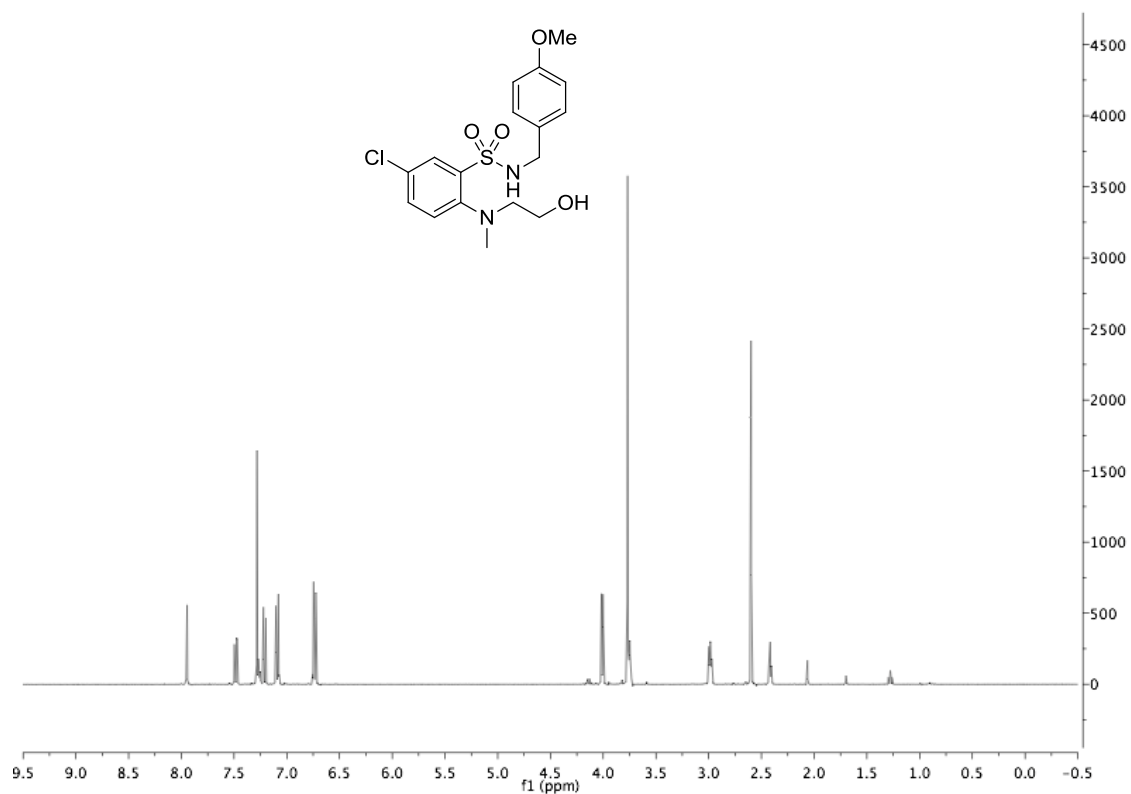
## 1. NMR spectra

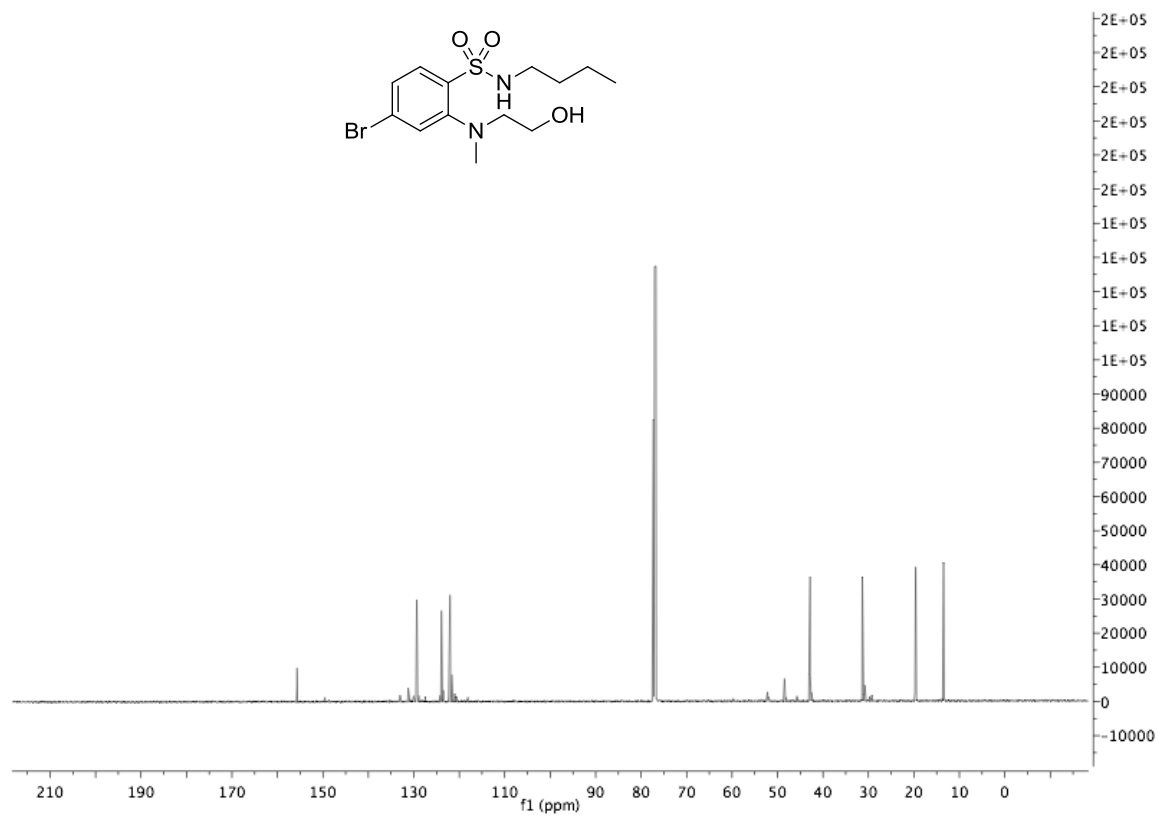
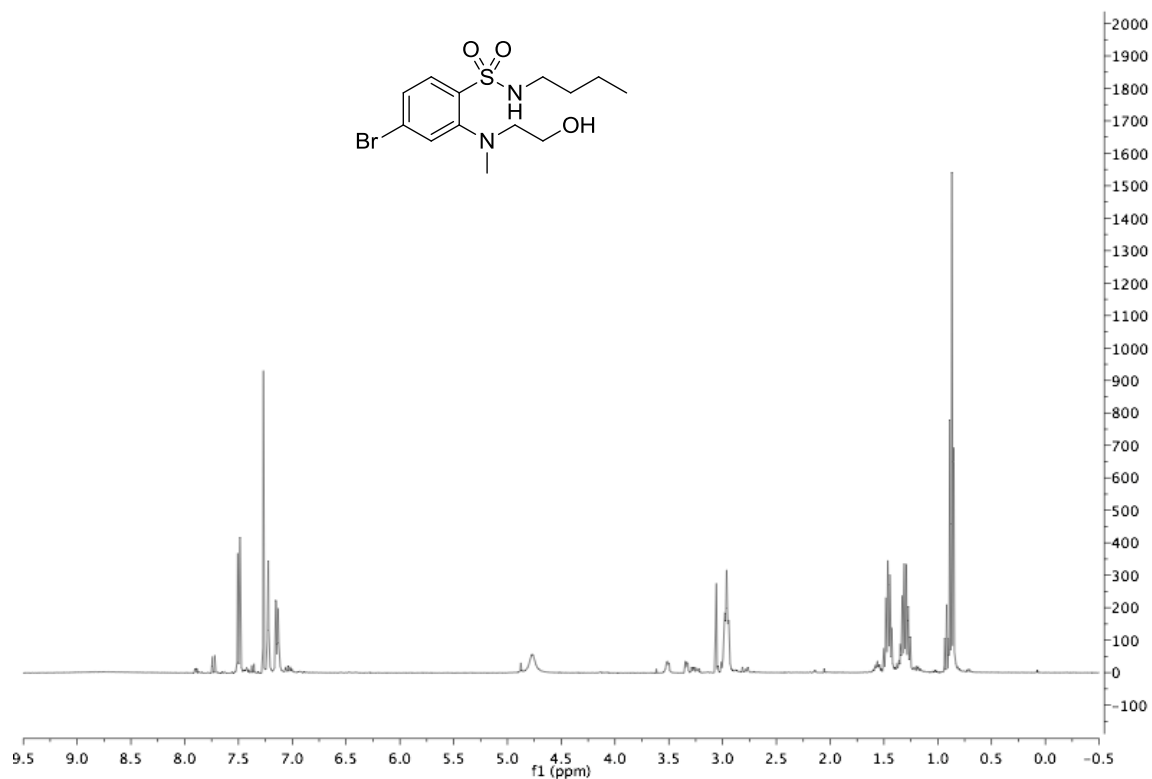
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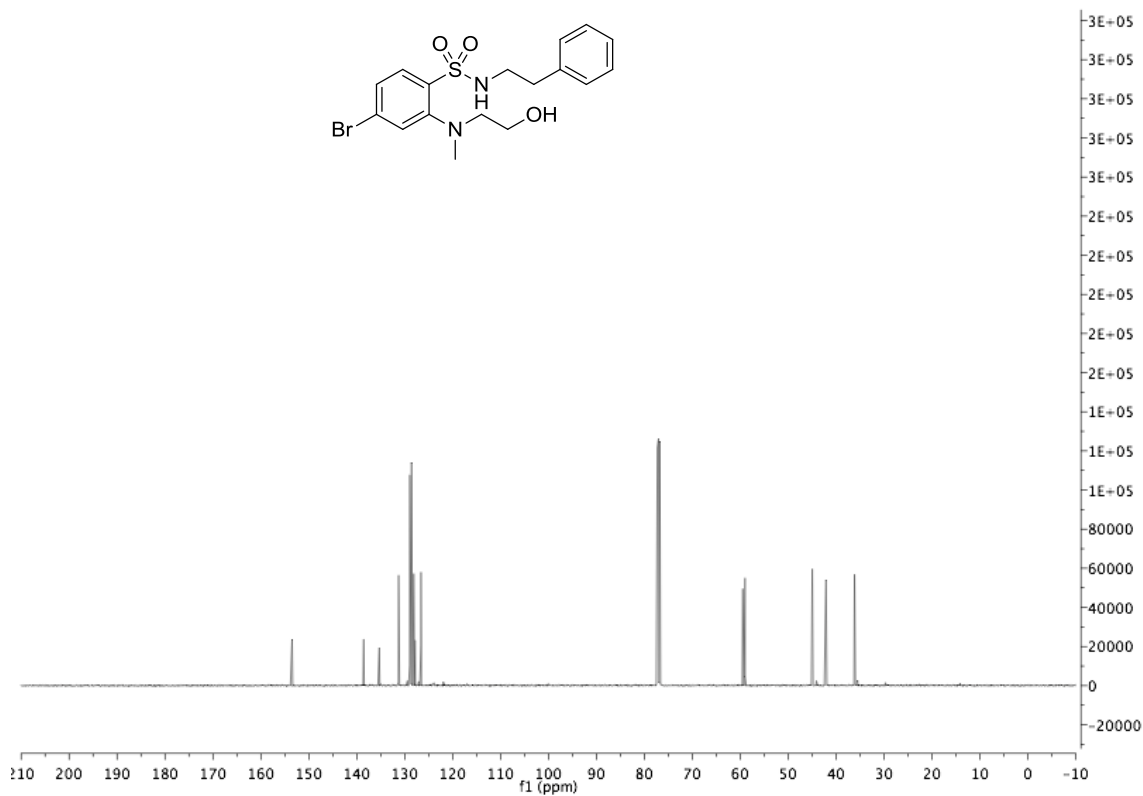
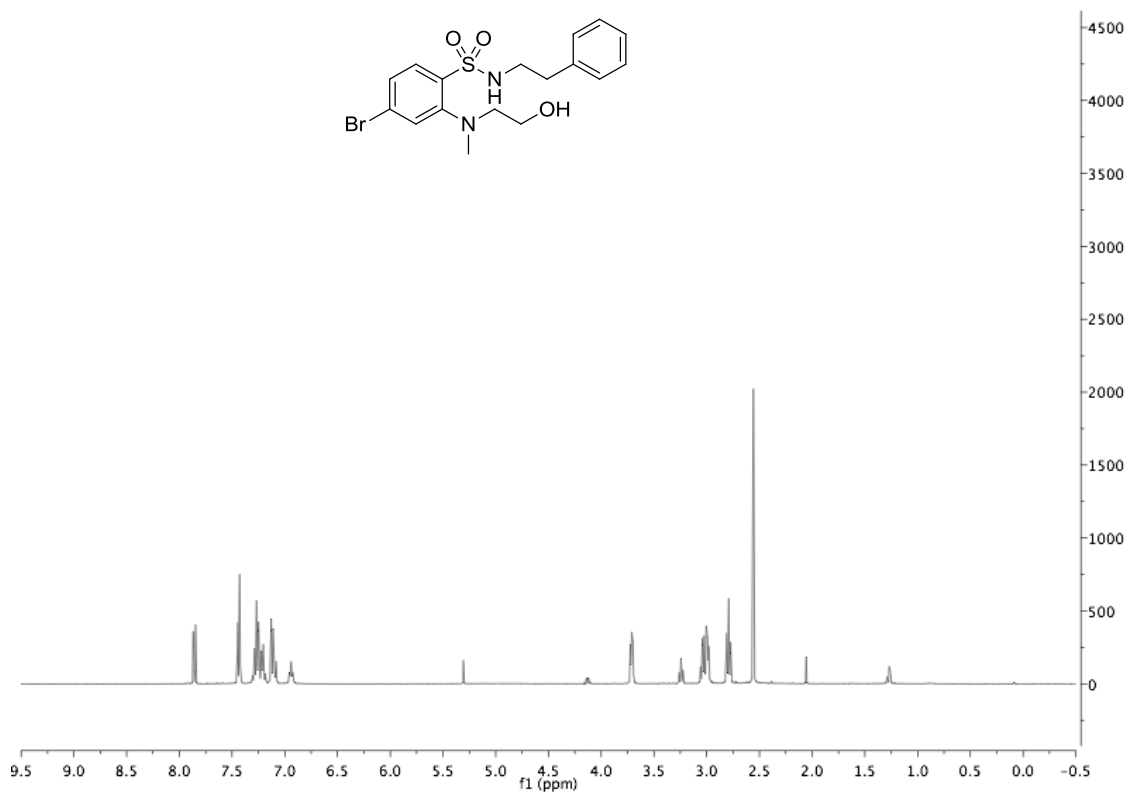


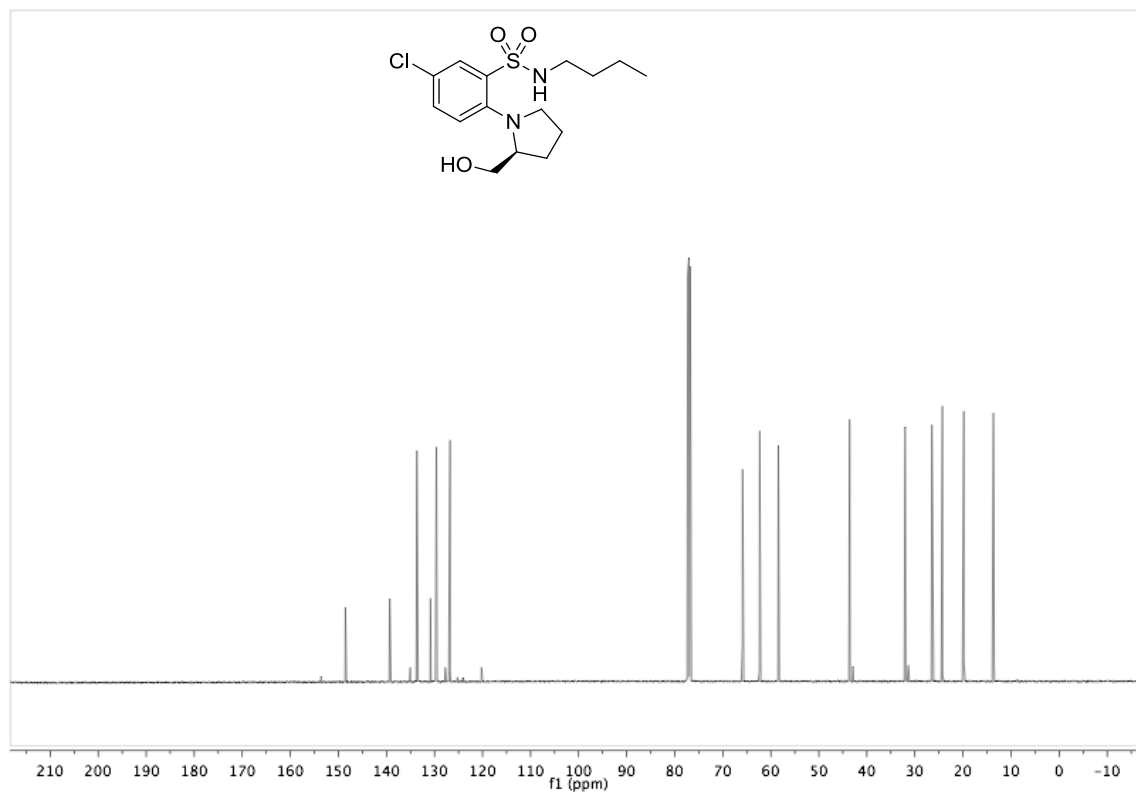
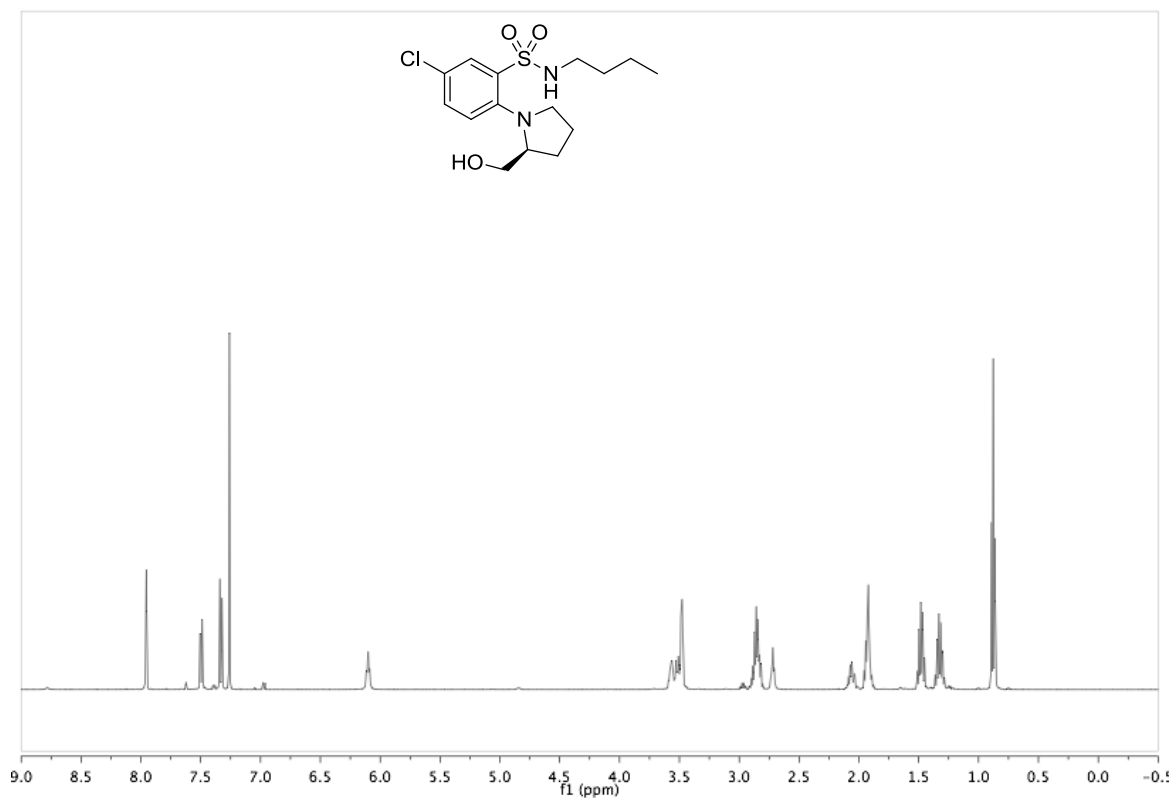
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**5-Chloro-*N*-cyclopentyl-2-((2-hydroxyethyl)(methyl)amino)benzenesulfon-amide (2c)**

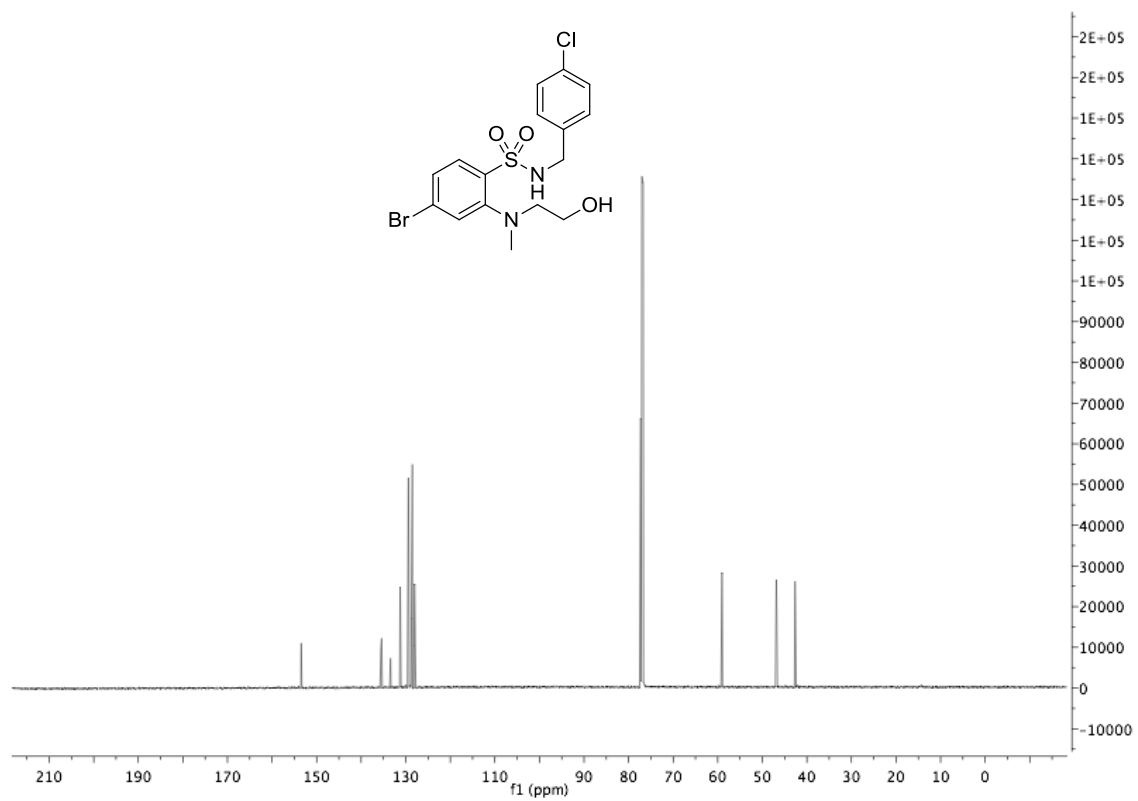
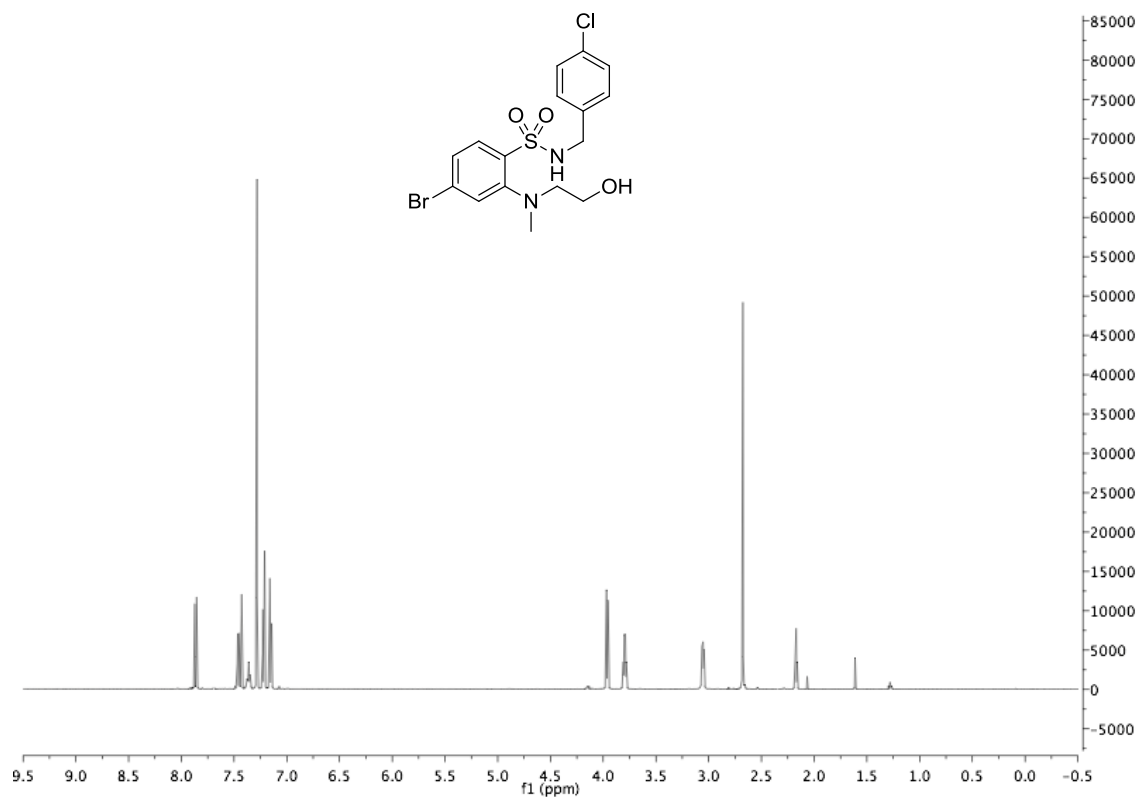
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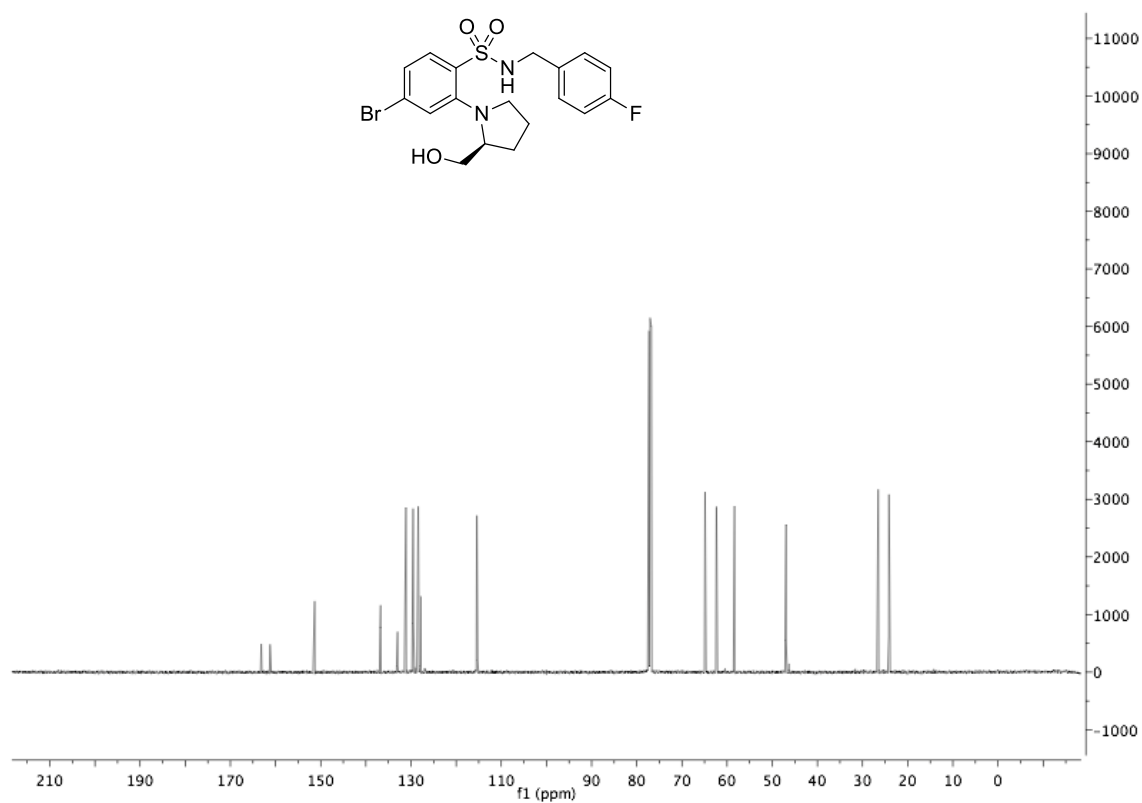
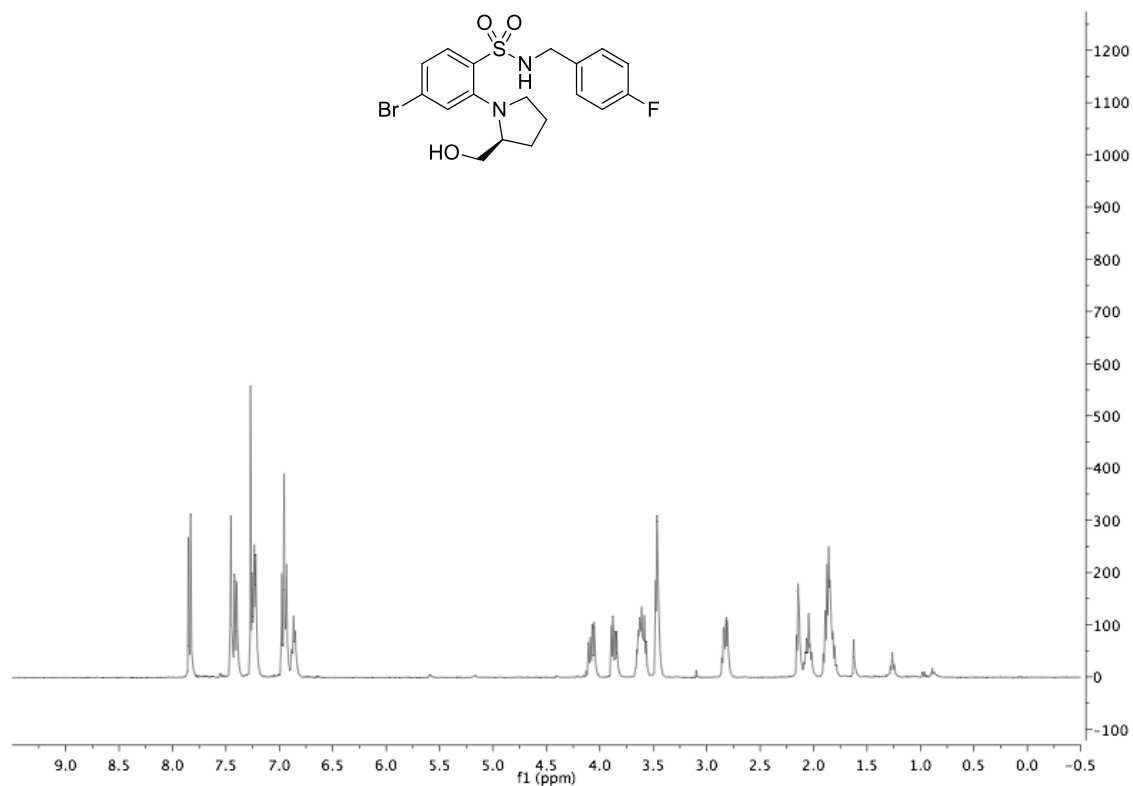
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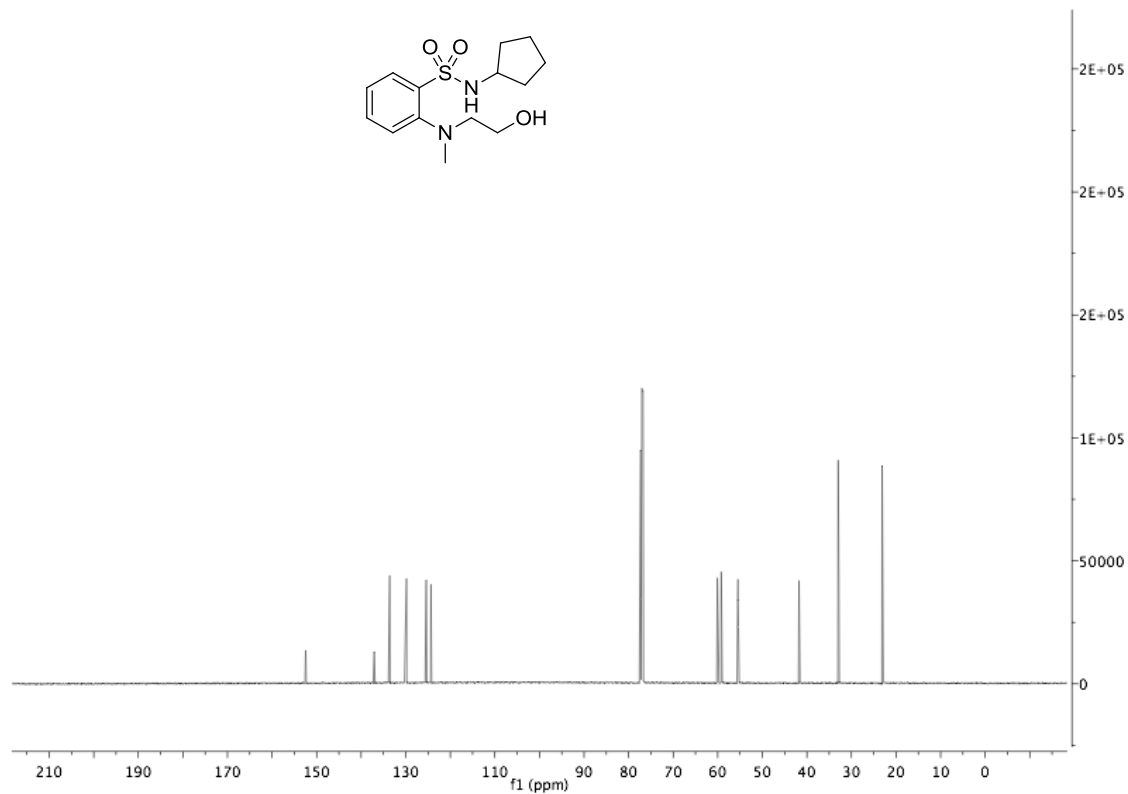
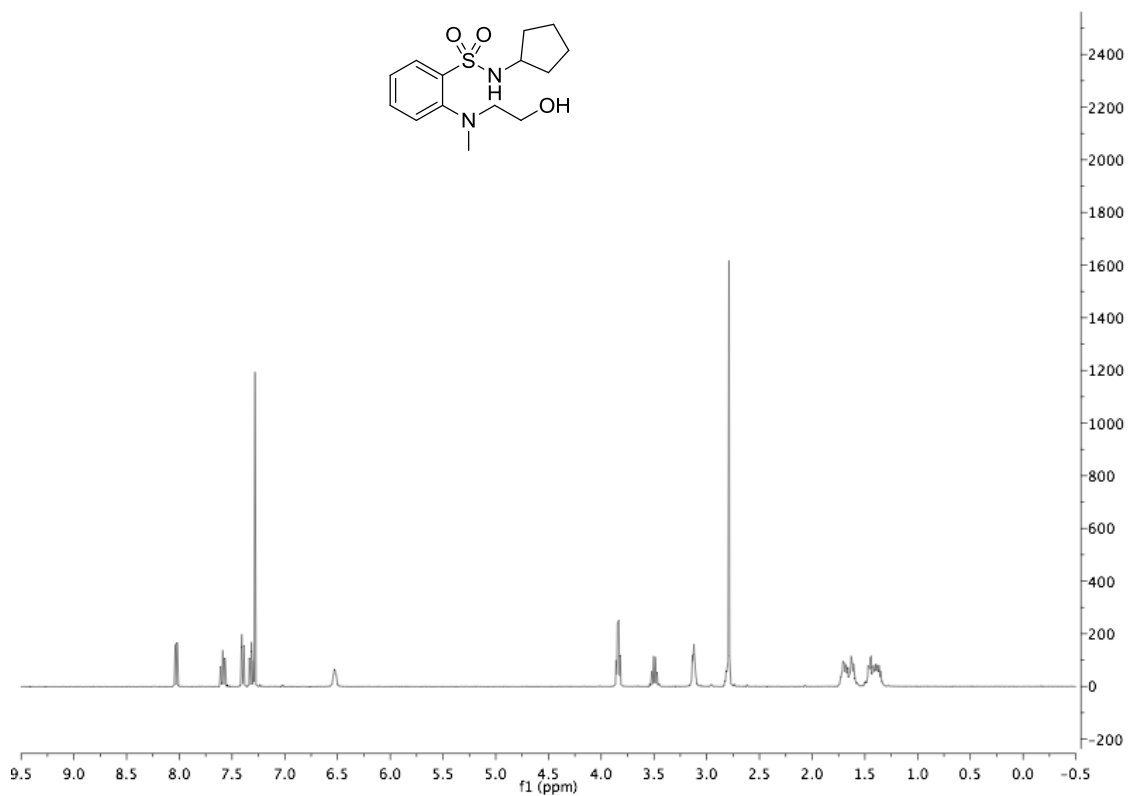
**4-Bromo-2-((2-hydroxyethyl)(methyl)amino)-*N*-phenethylbenzenesulfon-amide (2f)**

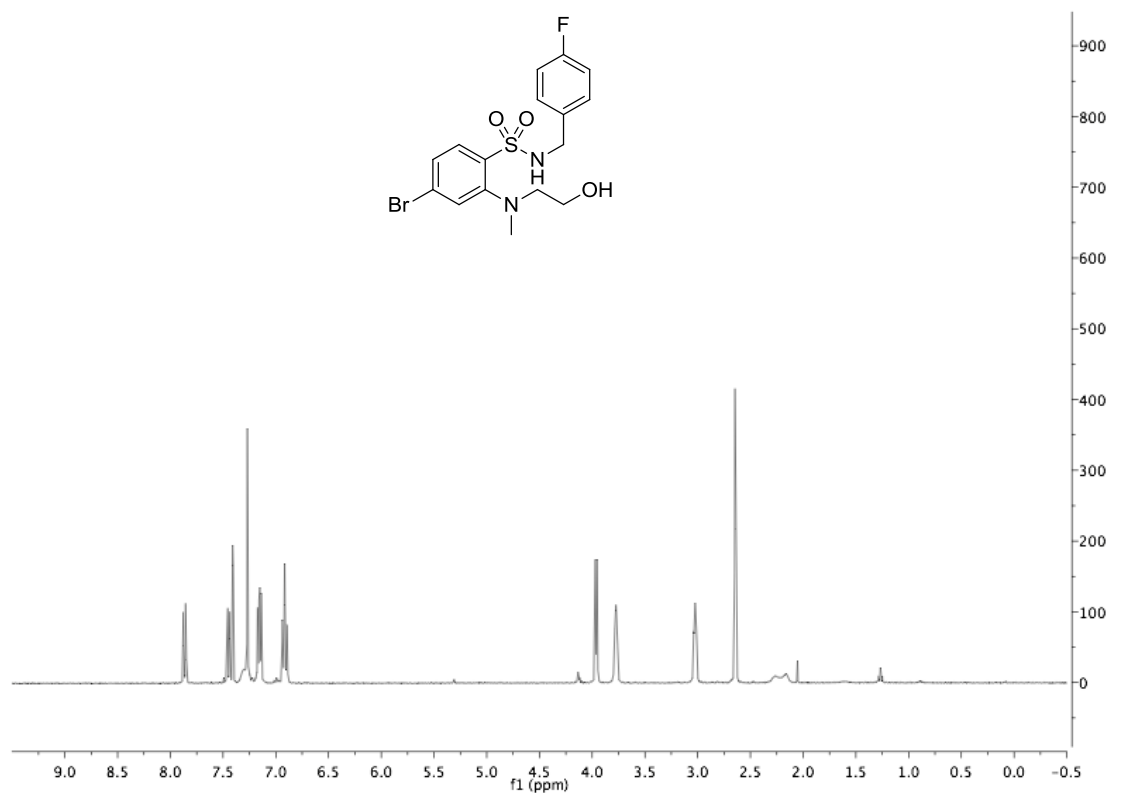
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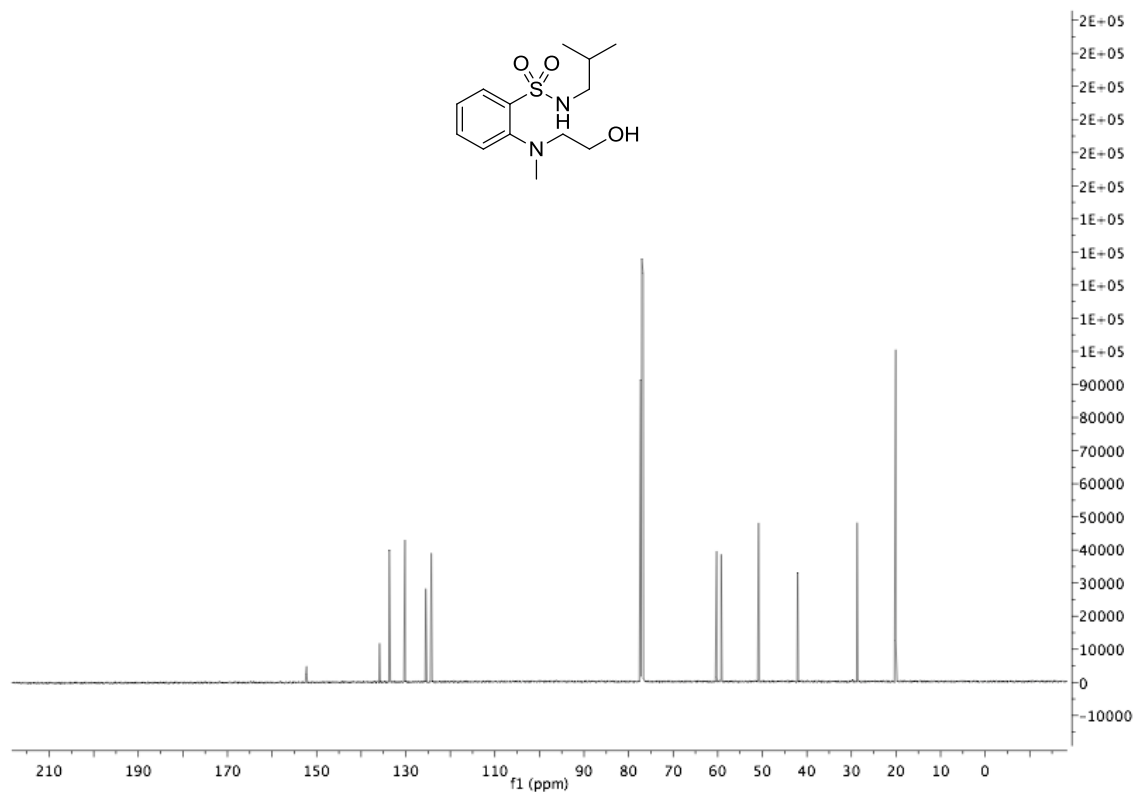
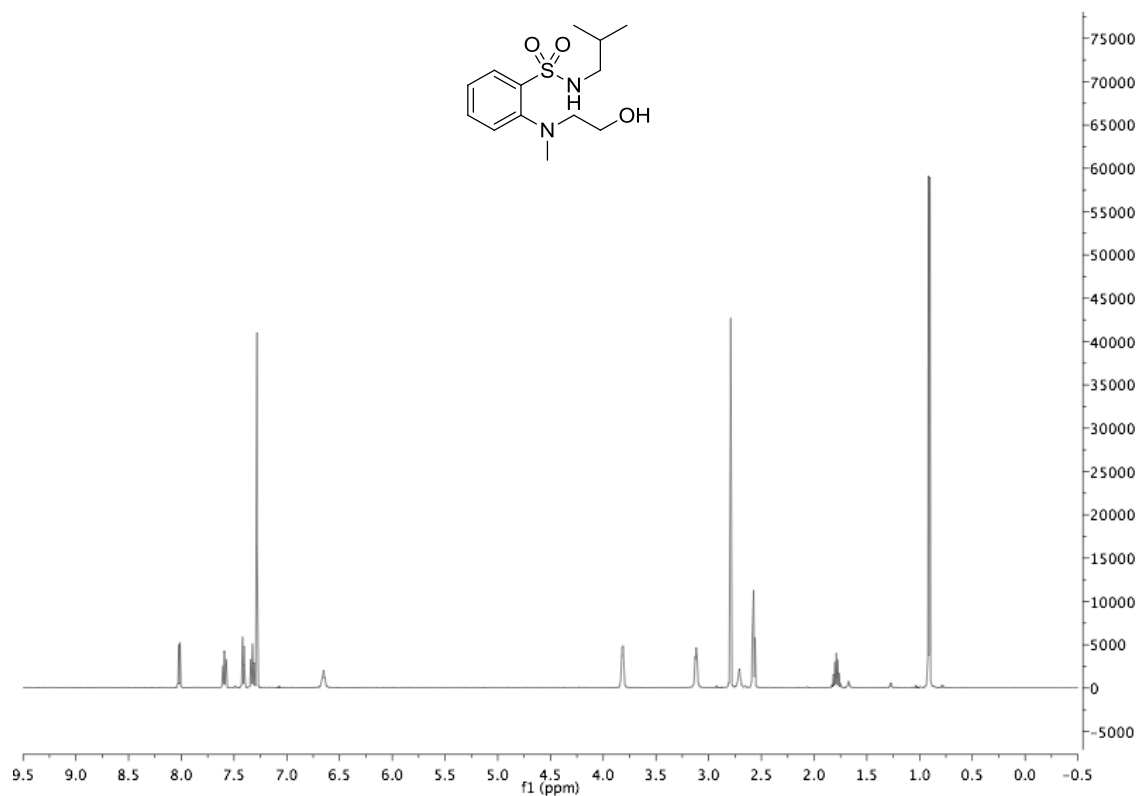


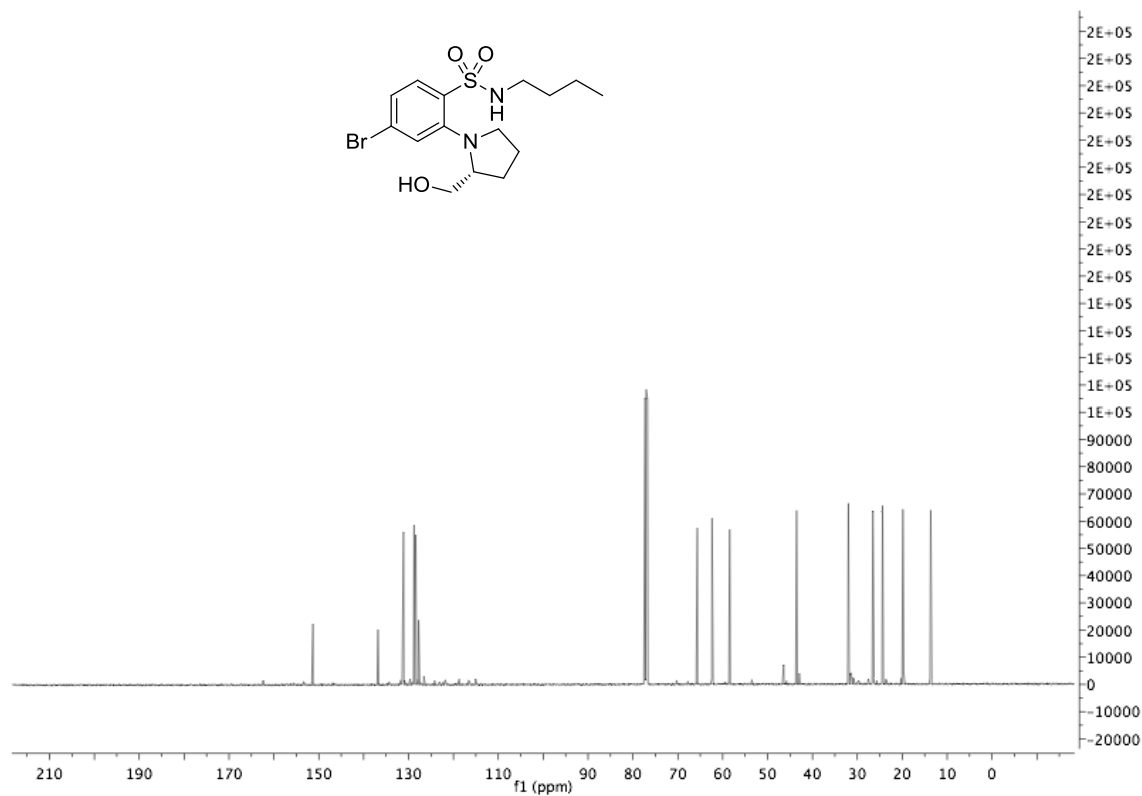
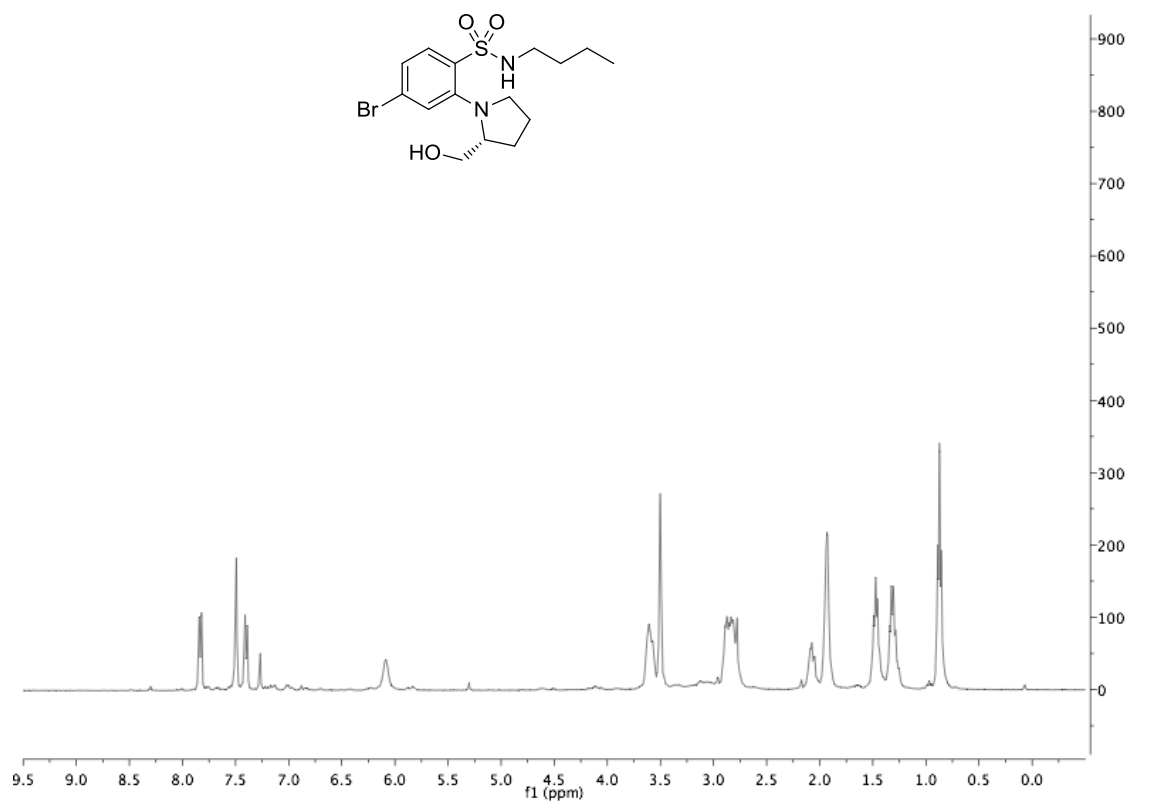
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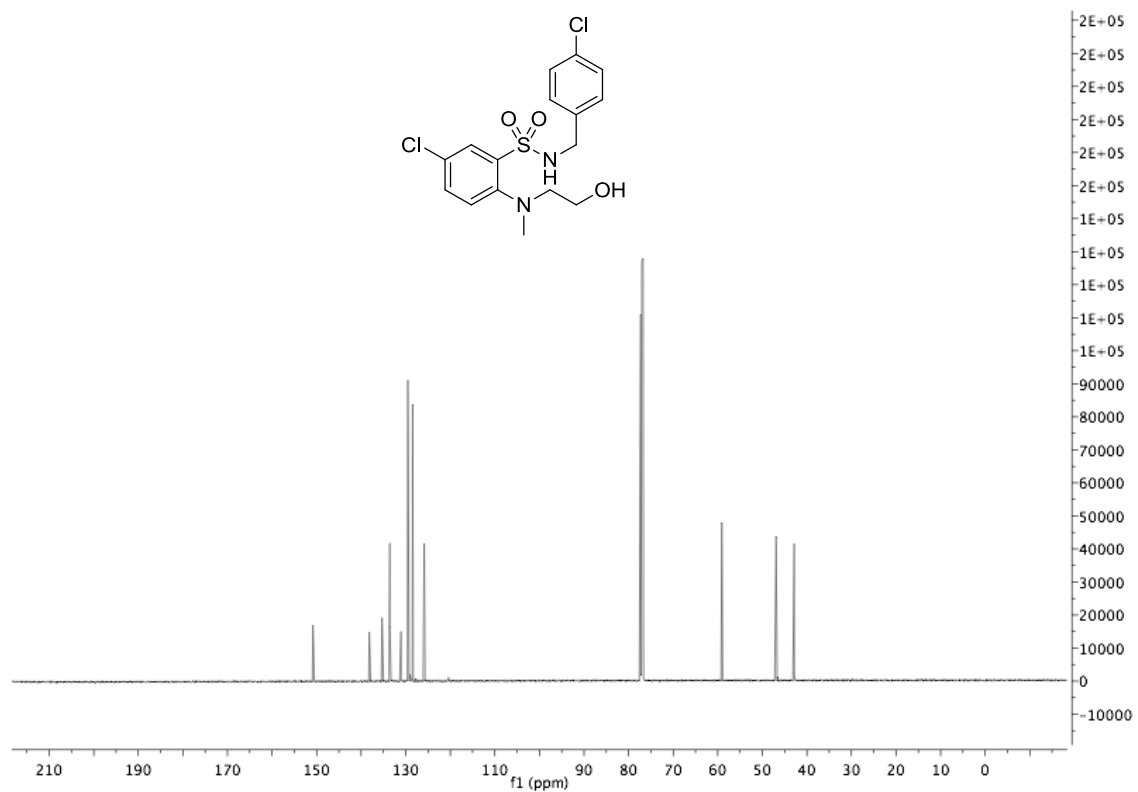
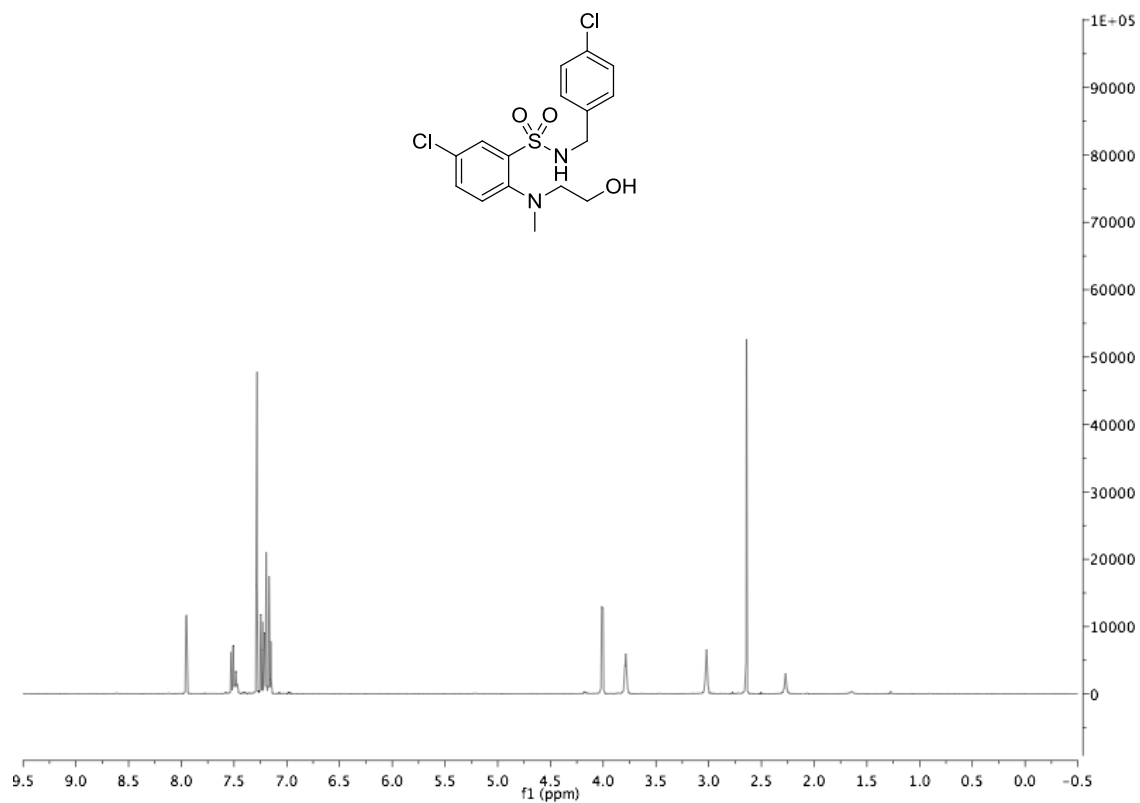
**(S)-4-Bromo-N-(4-fluorobenzyl)-2-(2-(hydroxymethyl)pyrrolidin-1-yl) benzenesulfonamide (2i)**

***N*-Cyclopentyl-2-((2-hydroxyethyl)(methyl)amino)benzenesulfonamide (2j)**

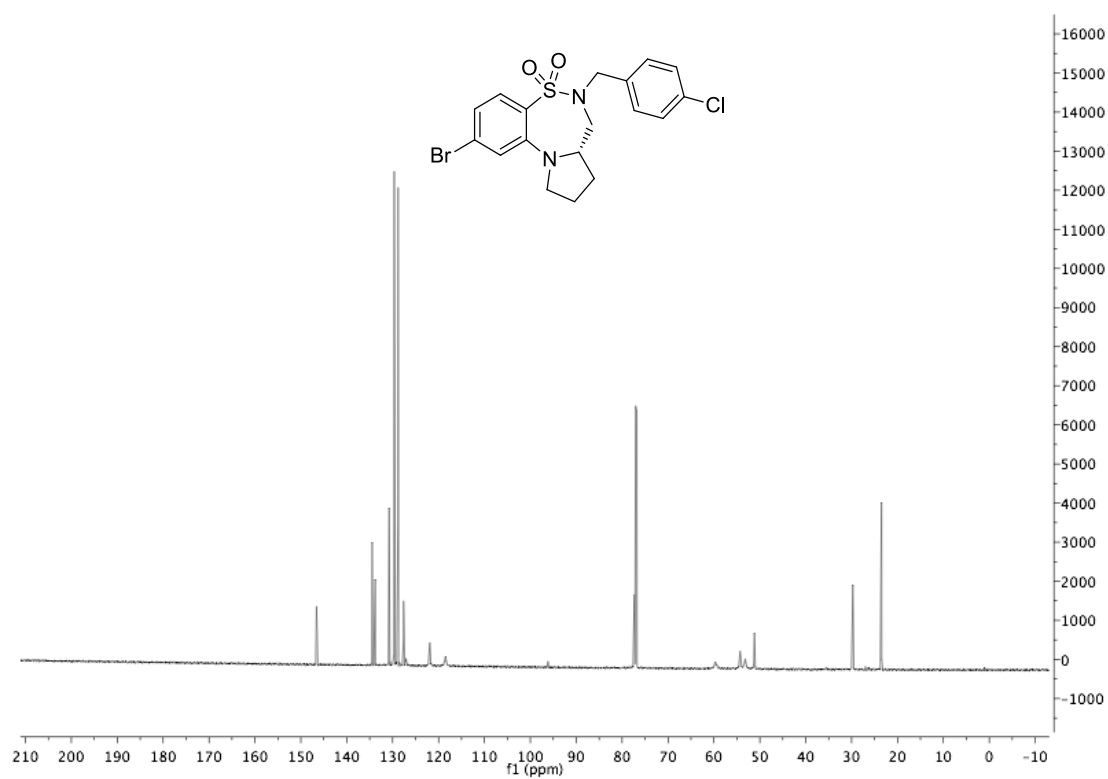
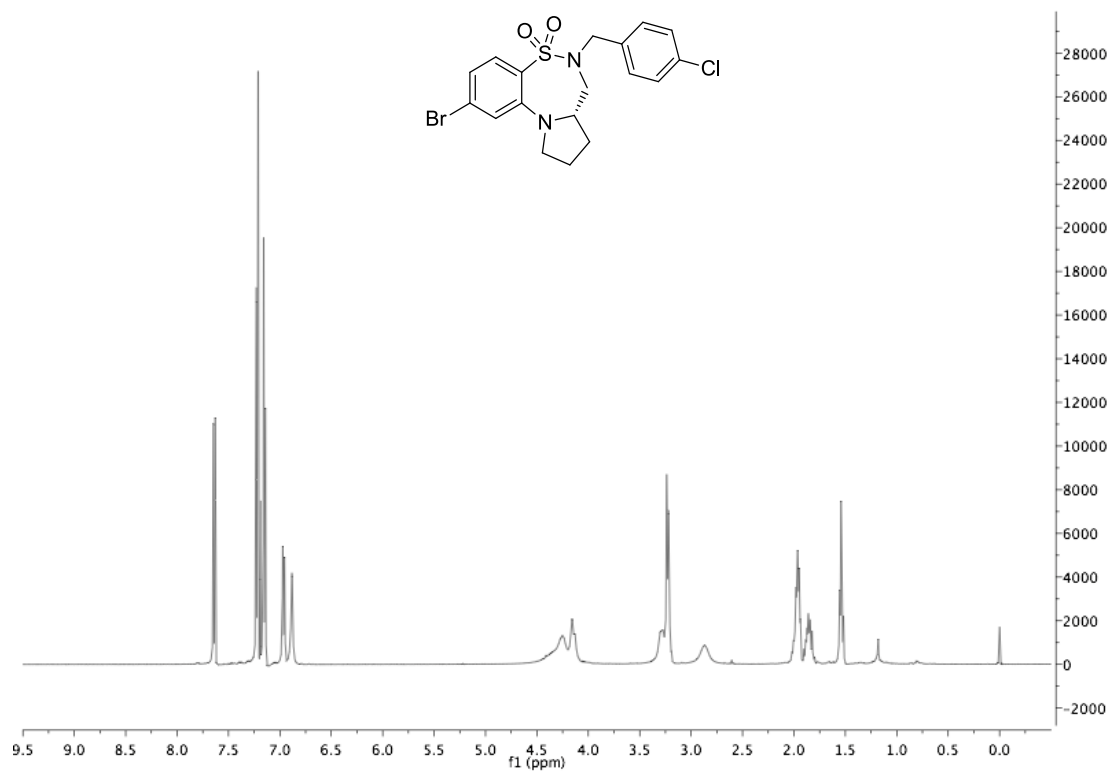
**4-Bromo-*N*-(4-fluorobenzyl)-2-((2-hydroxyethyl)(methyl)amino)benzene-sulfonamide (2k)**

**2-((2-Hydroxyethyl)(methyl)amino)-*N*-isobutylbenzenesulfonamide (2I)**

**(R)-4-Bromo-N-butyl-2-(2-(hydroxymethyl)pyrrolidin-1-yl)benzenesulfon-amide (2m)**

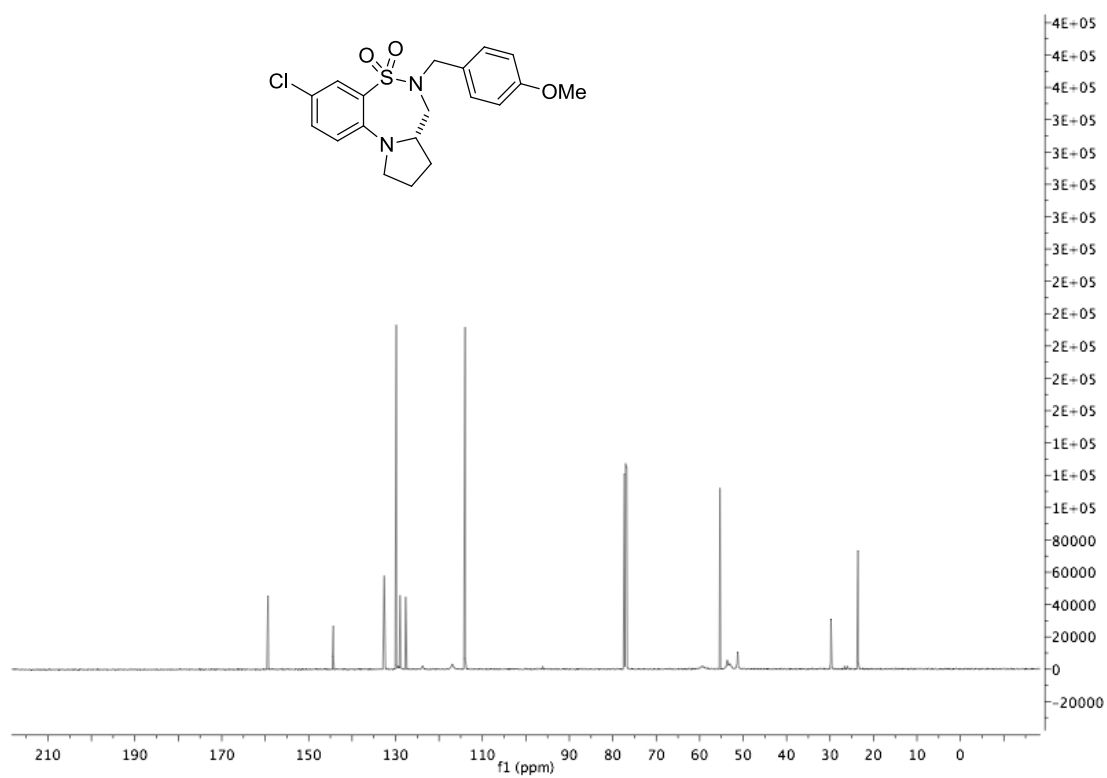
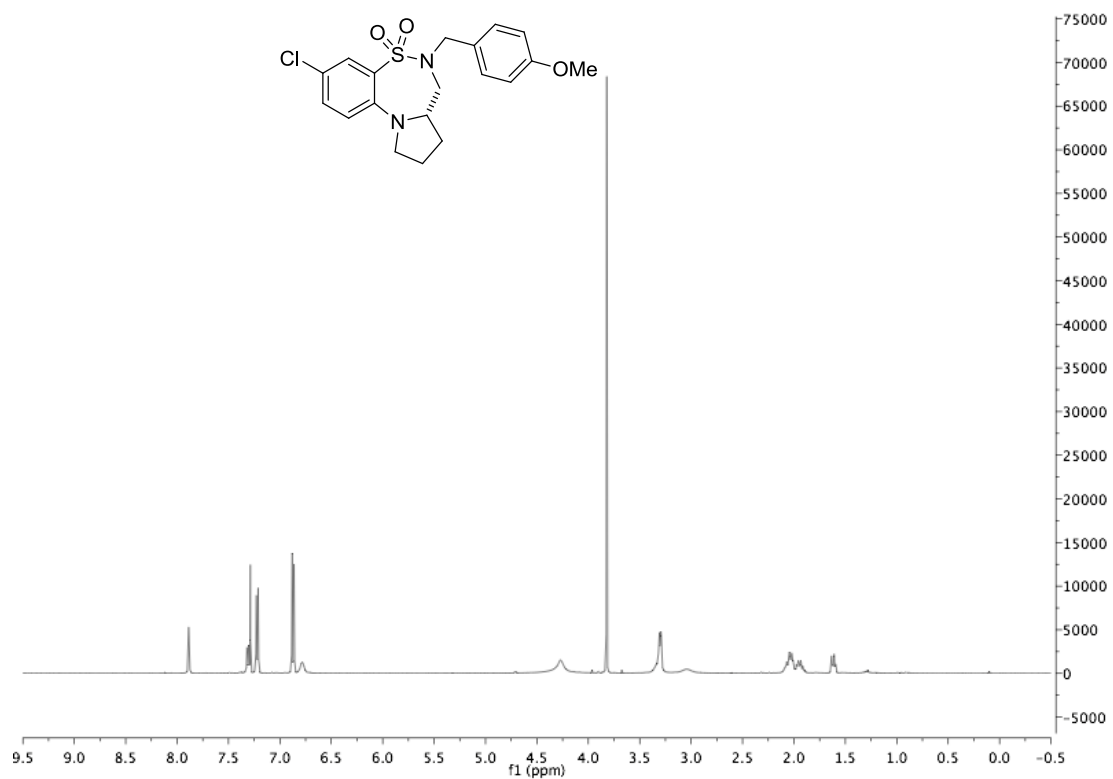
**5-Chloro-*N*-(4-chlorobenzyl)-2-((2-hydroxyethyl)(methyl)amino)benzene-sulfonamide (2n)**

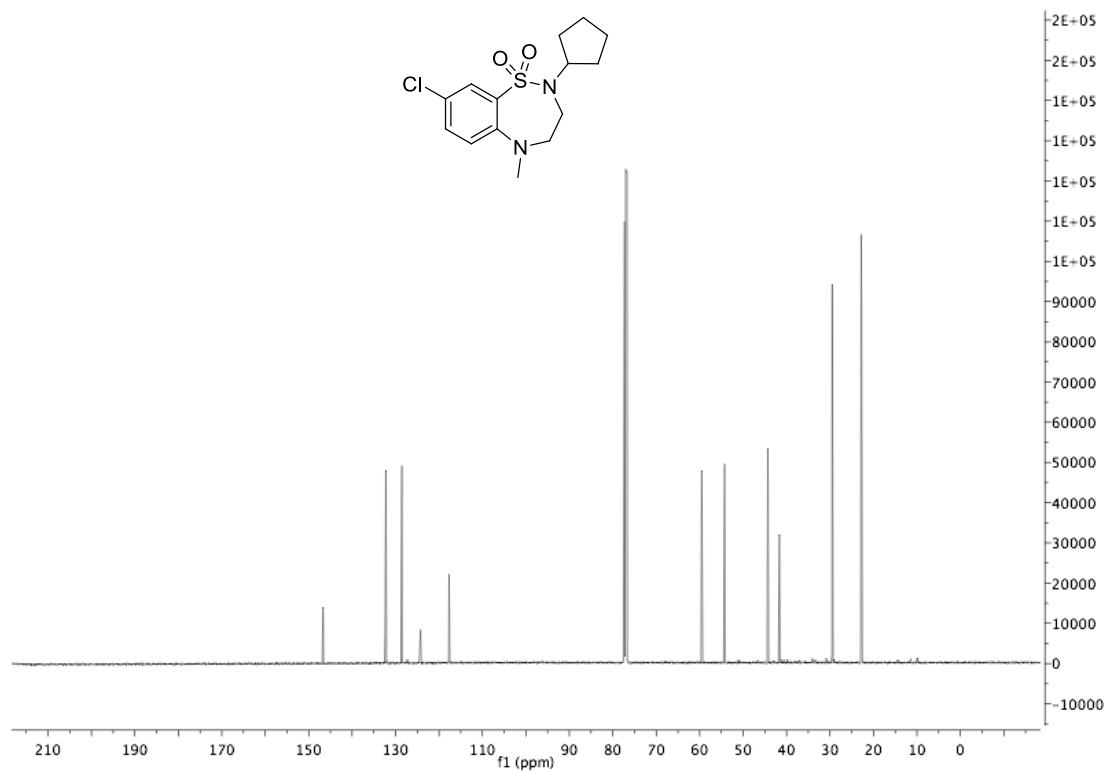
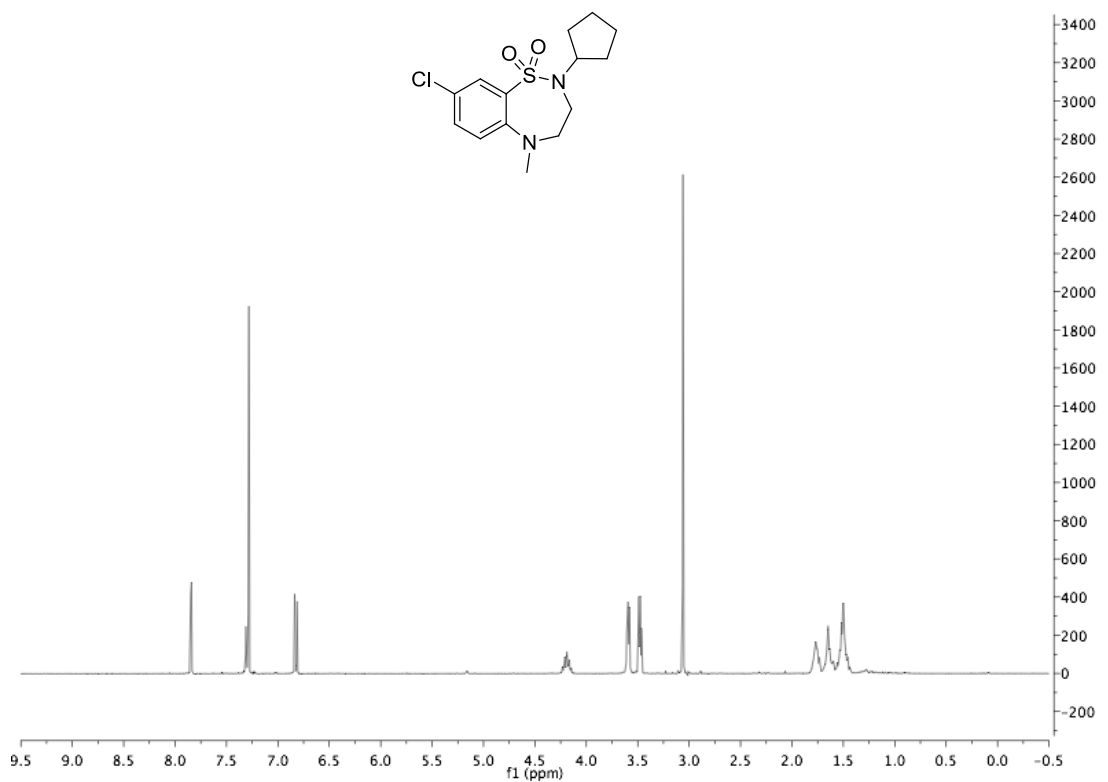
**(S)-2-Bromo-6-(4-chlorobenzyl)-6,7,7a,8,9,10-hexahydrobenzo[*f*] pyrrolo-[2,1-*d*][1,2,5]thiadiazepine 5,5-dioxide (3a)**

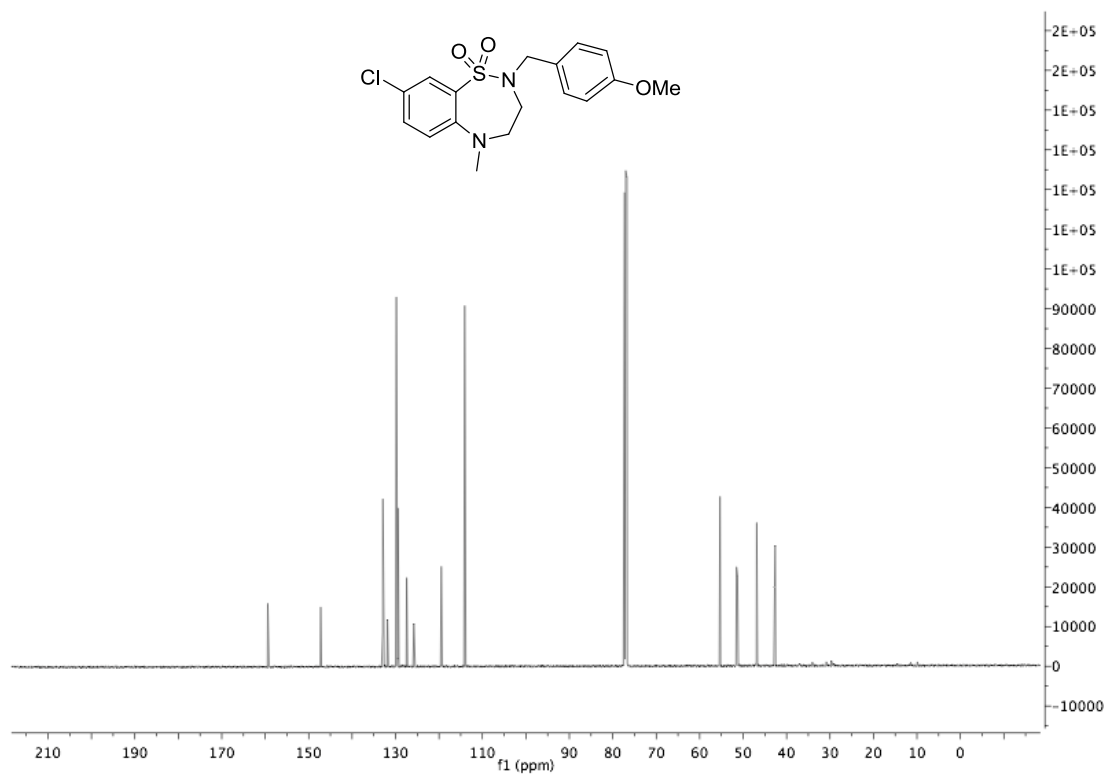
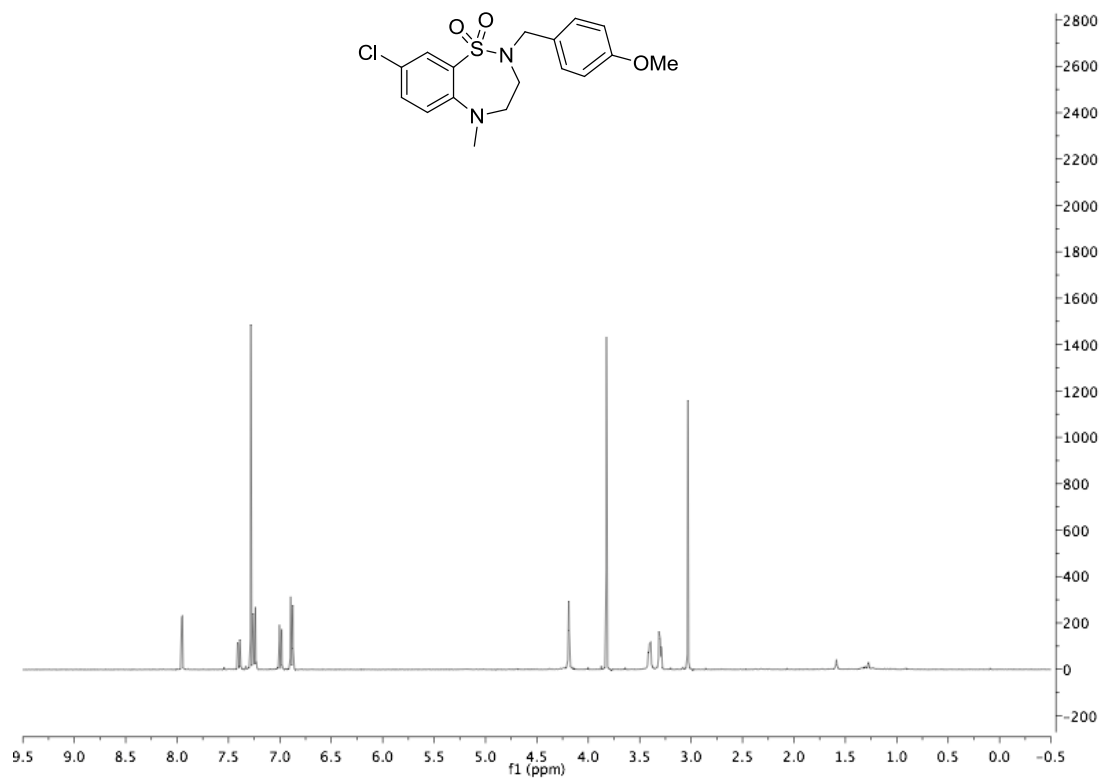


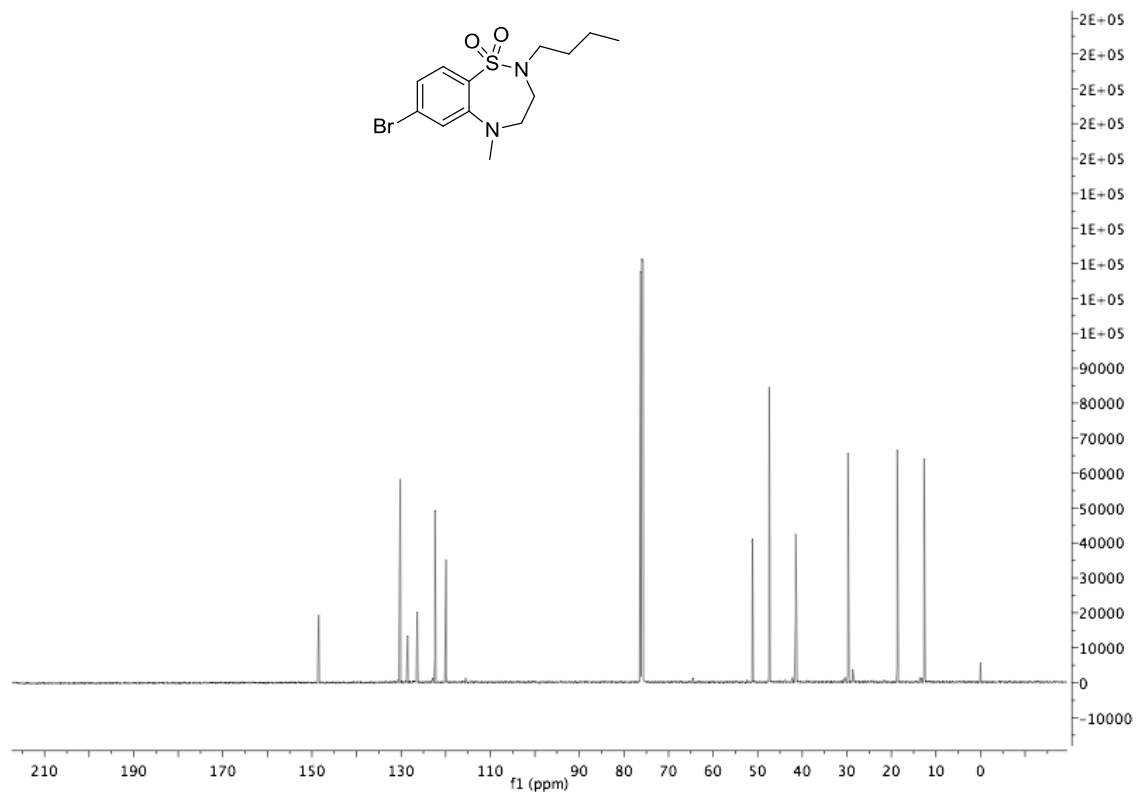
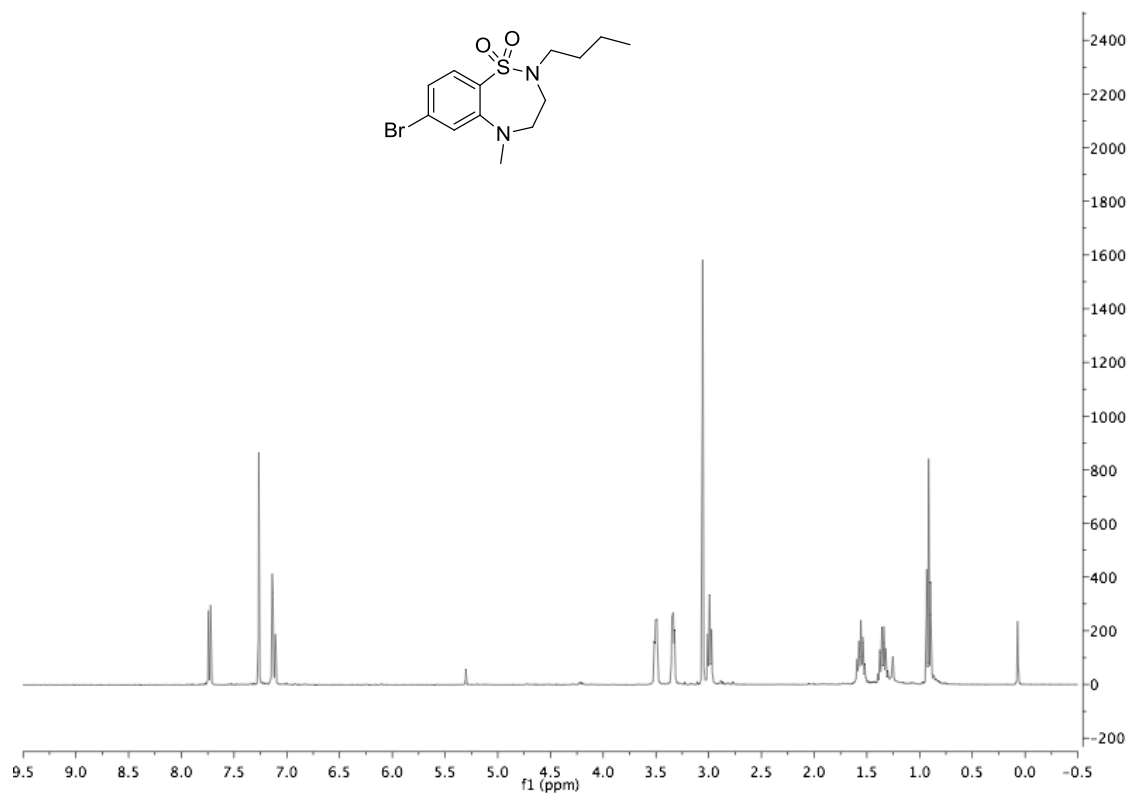


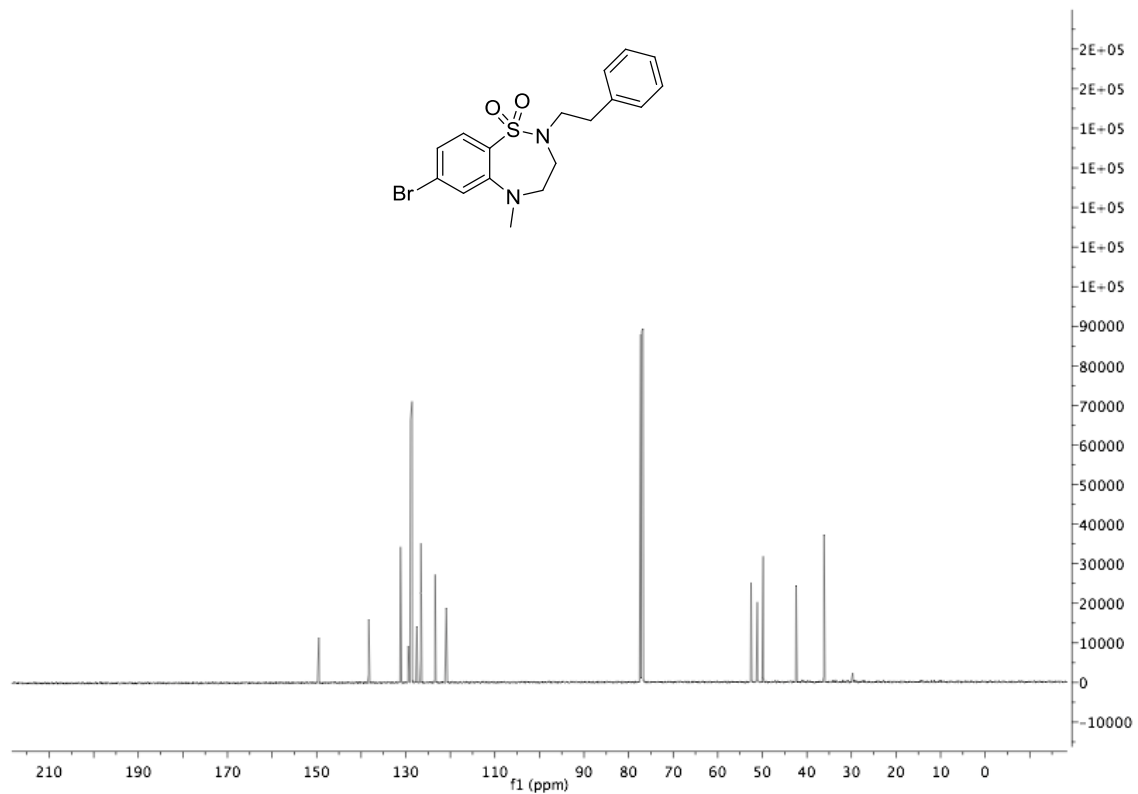
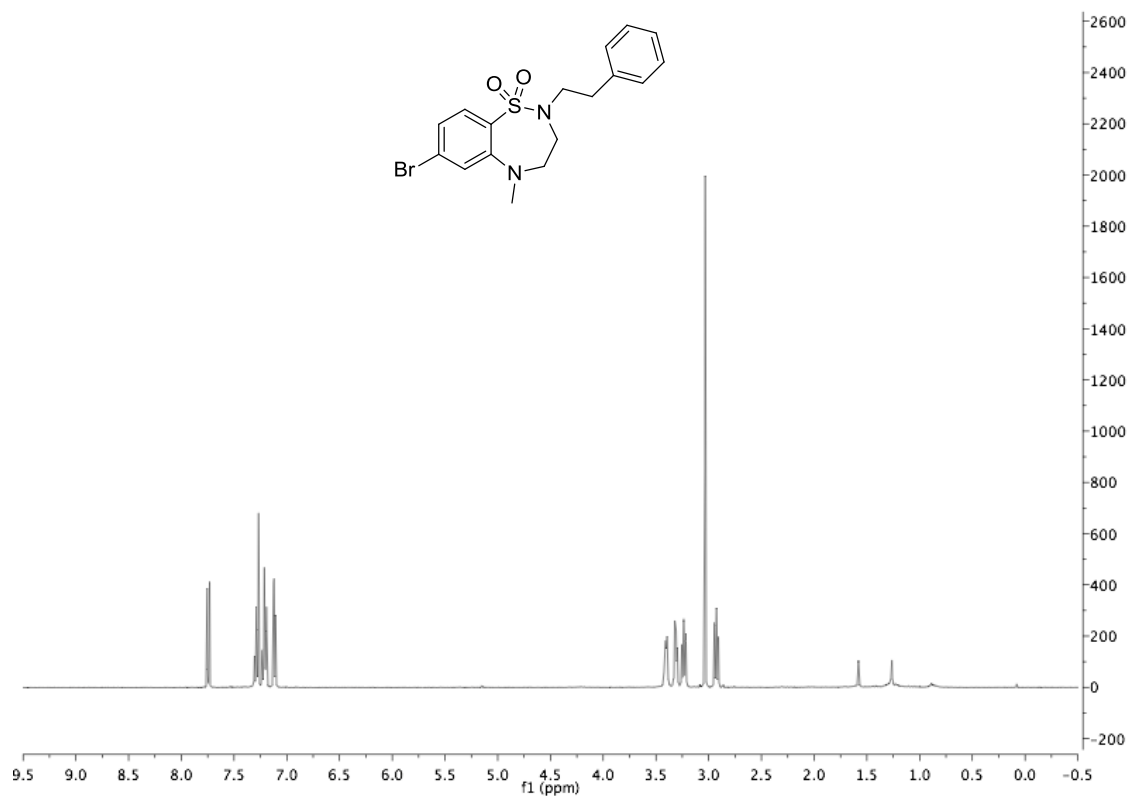
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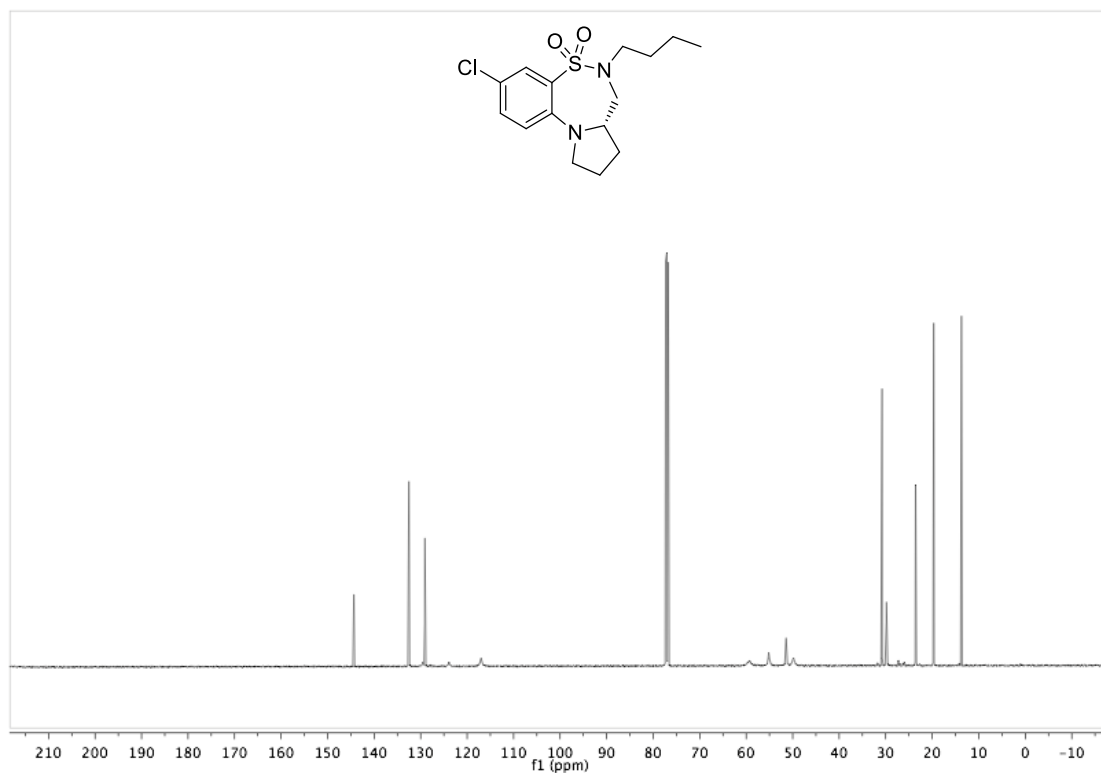
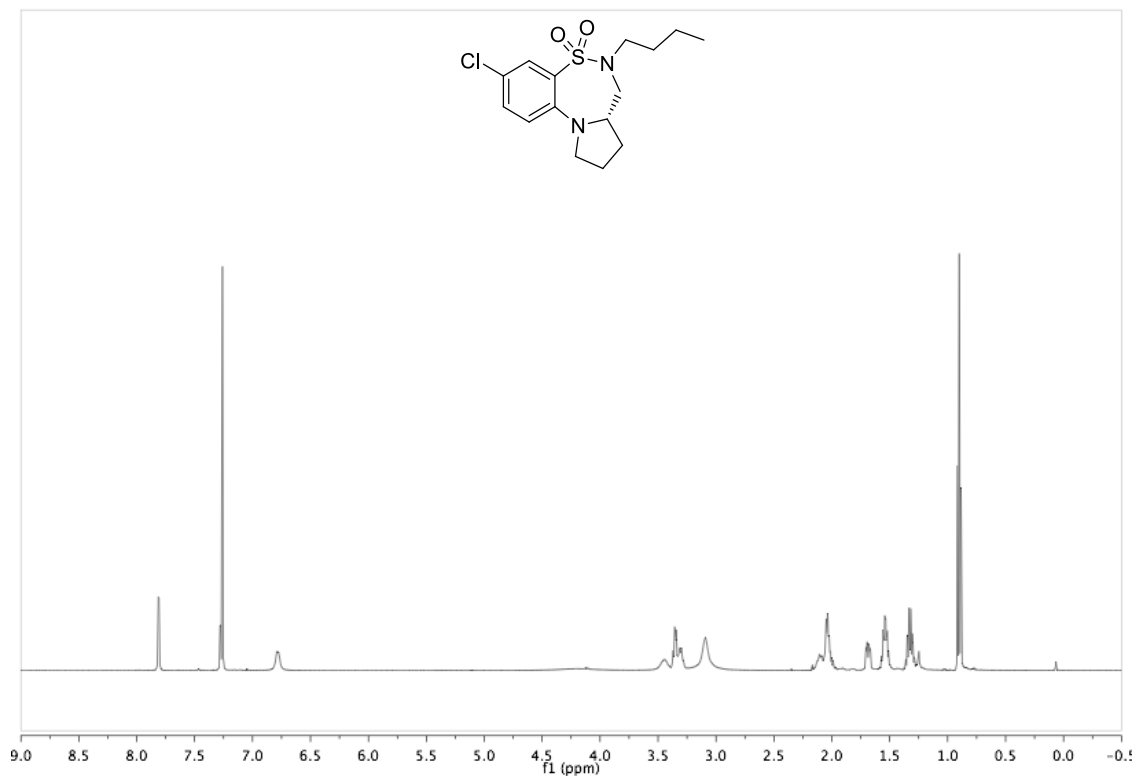
**8-Chloro-2-cyclopentyl-5-methyl-2,3,4,5-tetrahydrobenzo[f][1,2,5] thiadiazepine 1,1-dioxide (3c)**

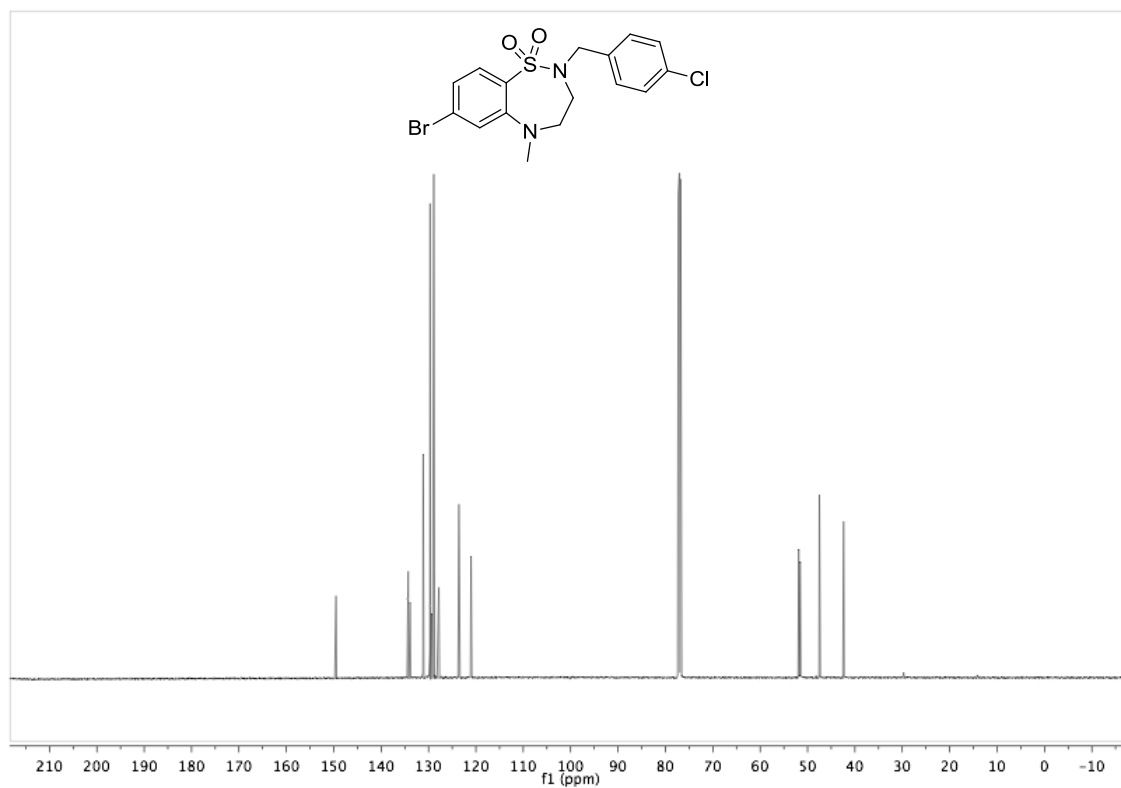
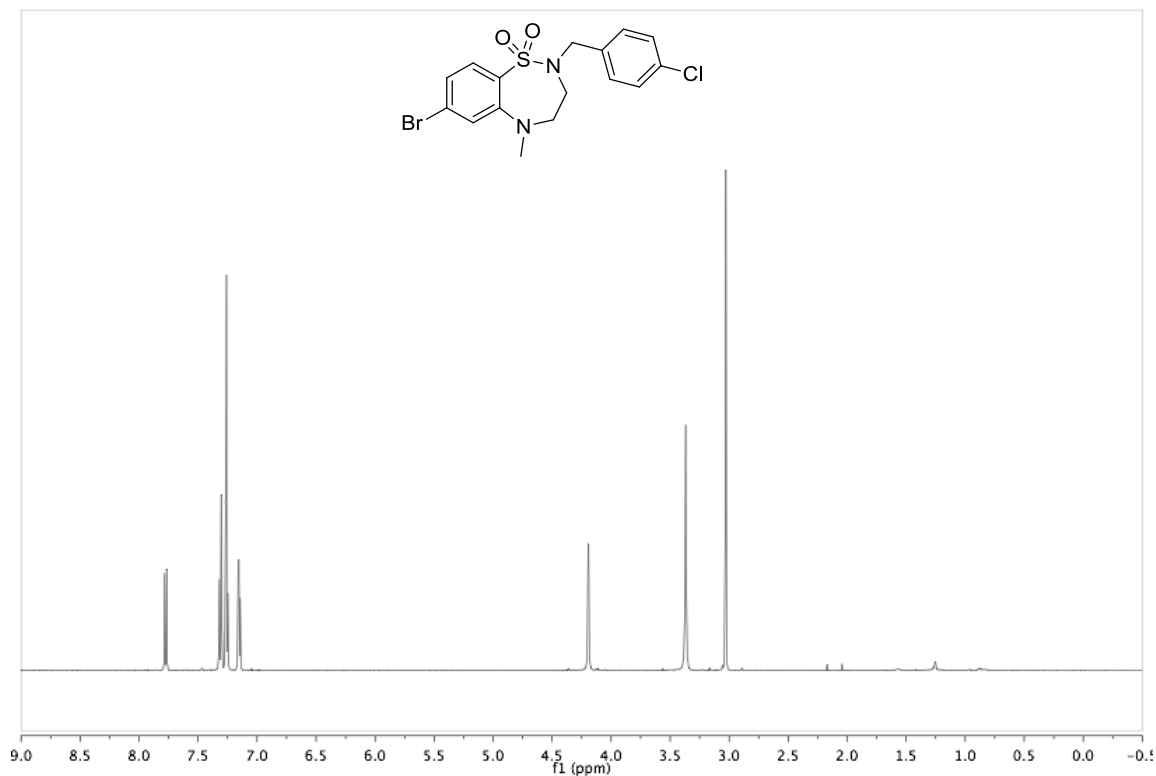
**8-Chloro-2-(4-methoxybenzyl)-5-methyl-2,3,4,5-tetrahydrobenzo[f][1,2,5] thiadiazepine 1,1-dioxide (3d)**

**7-Bromo-2-butyl-5-methyl-2,3,4,5-tetrahydrobenzo[*f*][1,2,5]thiadiazepine 1,1-dioxide (3e)**

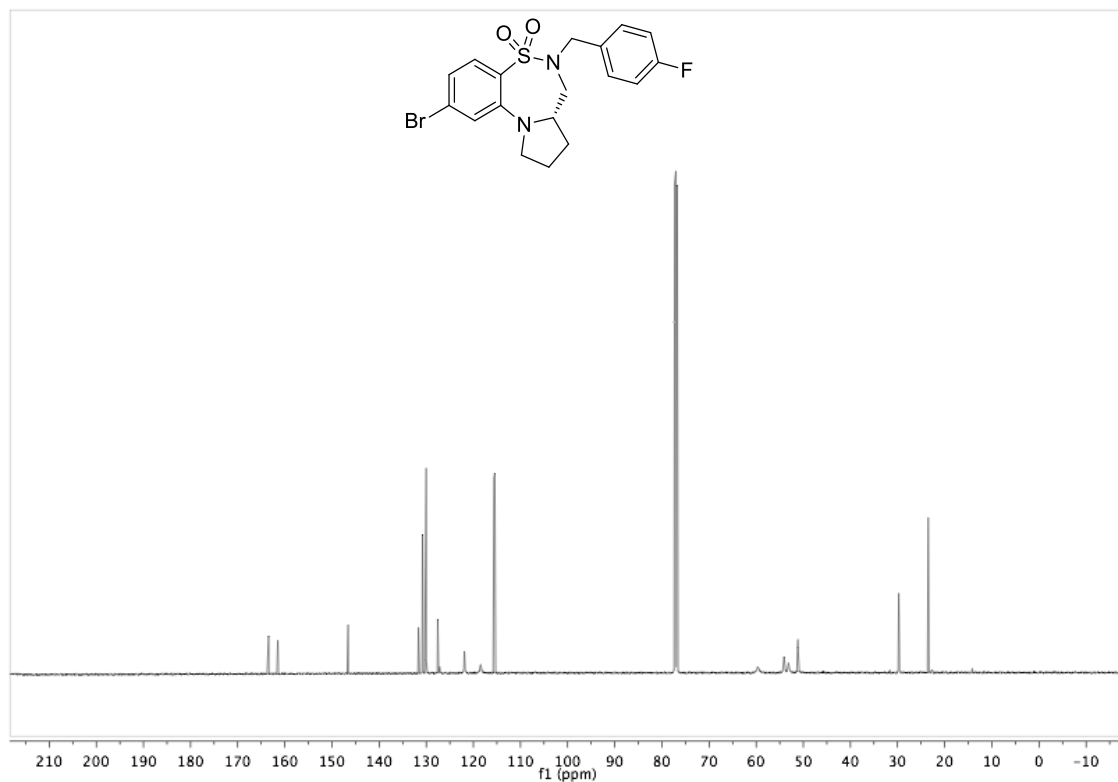
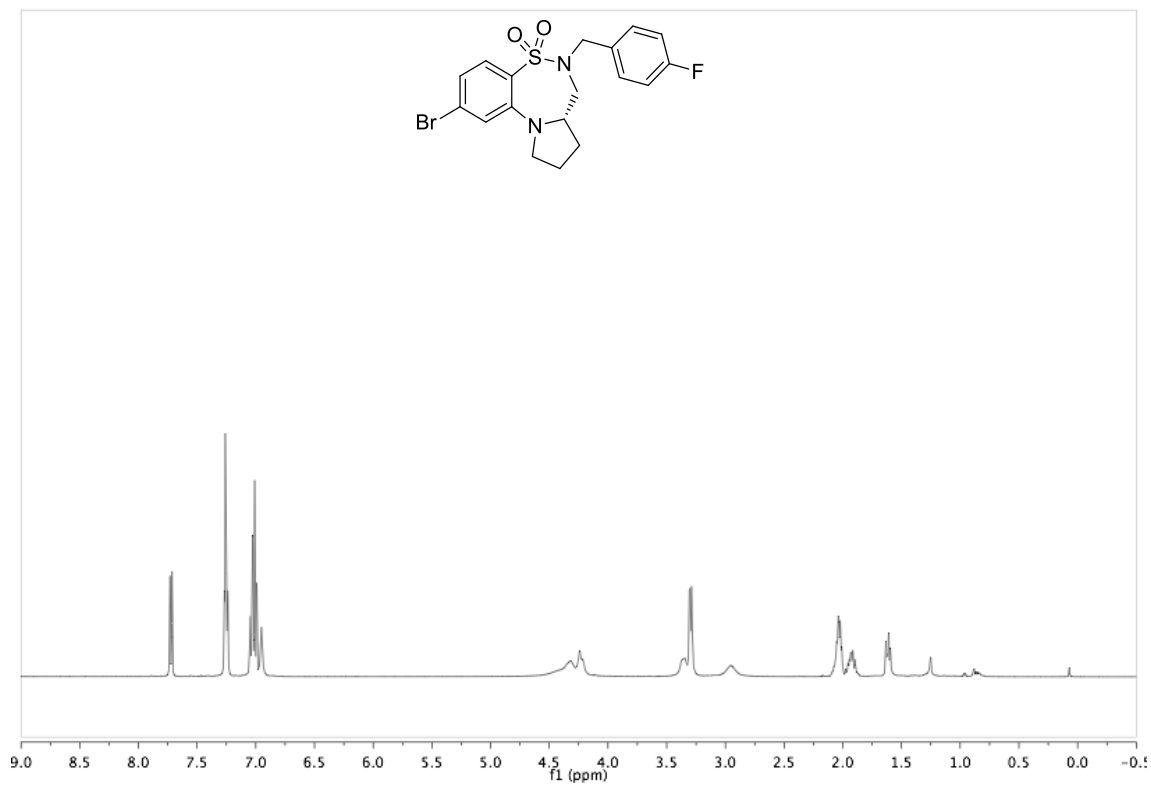
**7-Bromo-5-methyl-2-phenethyl-2,3,4,5-tetrahydrobenzo[*f*][1,2,5]thiadiazepine 1,1-dioxide (3f)**

**(S)-6-Butyl-3-chloro-6,7,7a,8,9,10-hexahydrobenzo[*f*]pyrrolo[2,1-*d*][1,2,5] thiadiazepine 5,5-dioxide (3g)**

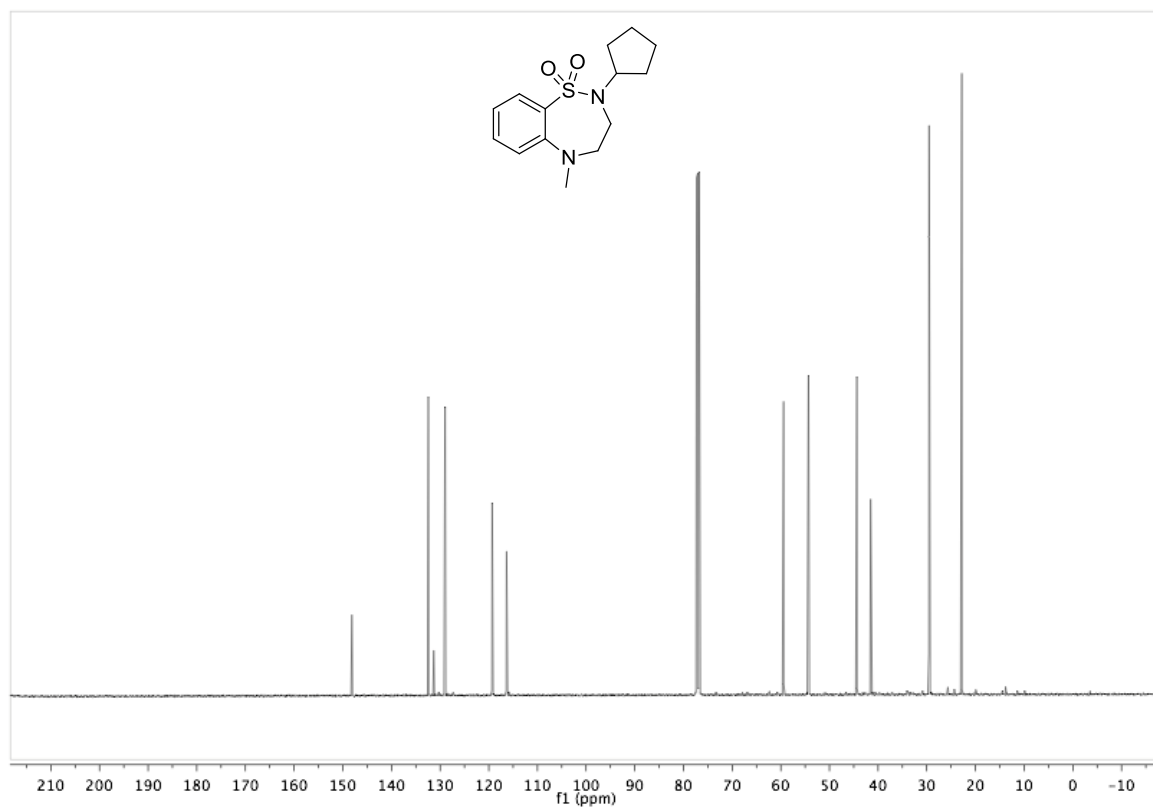
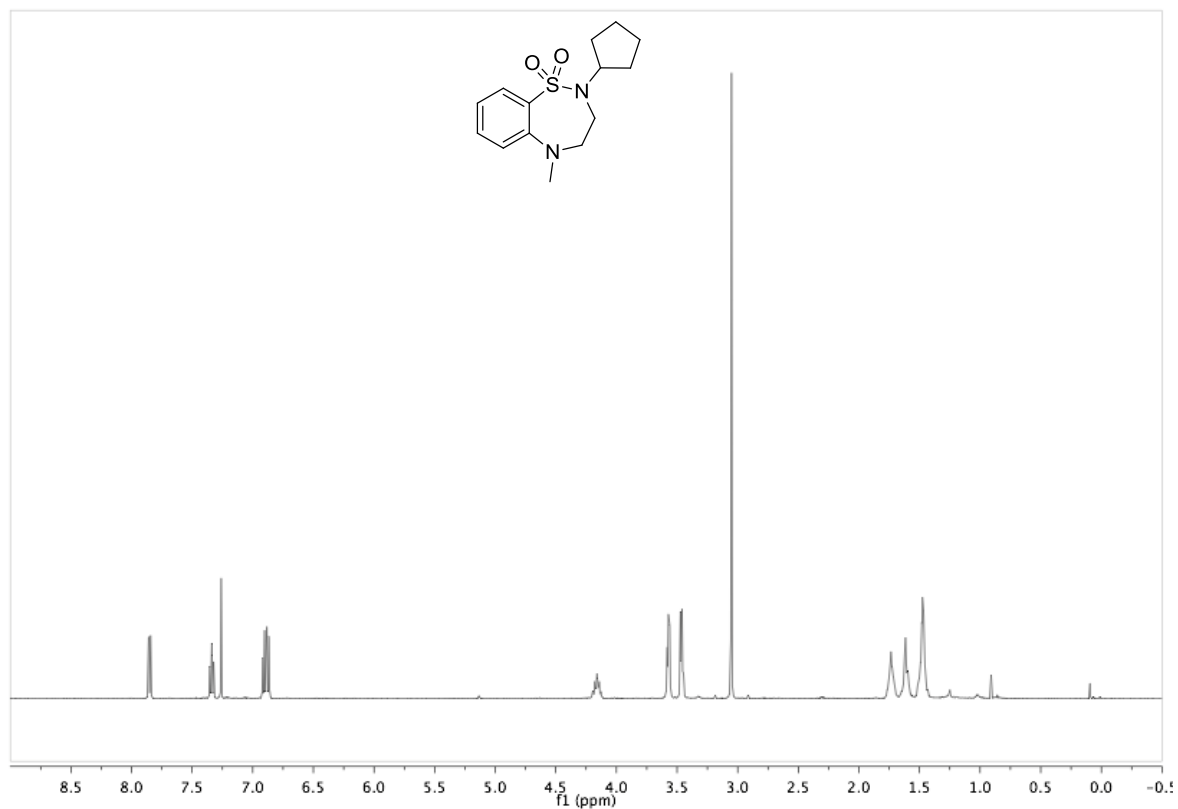


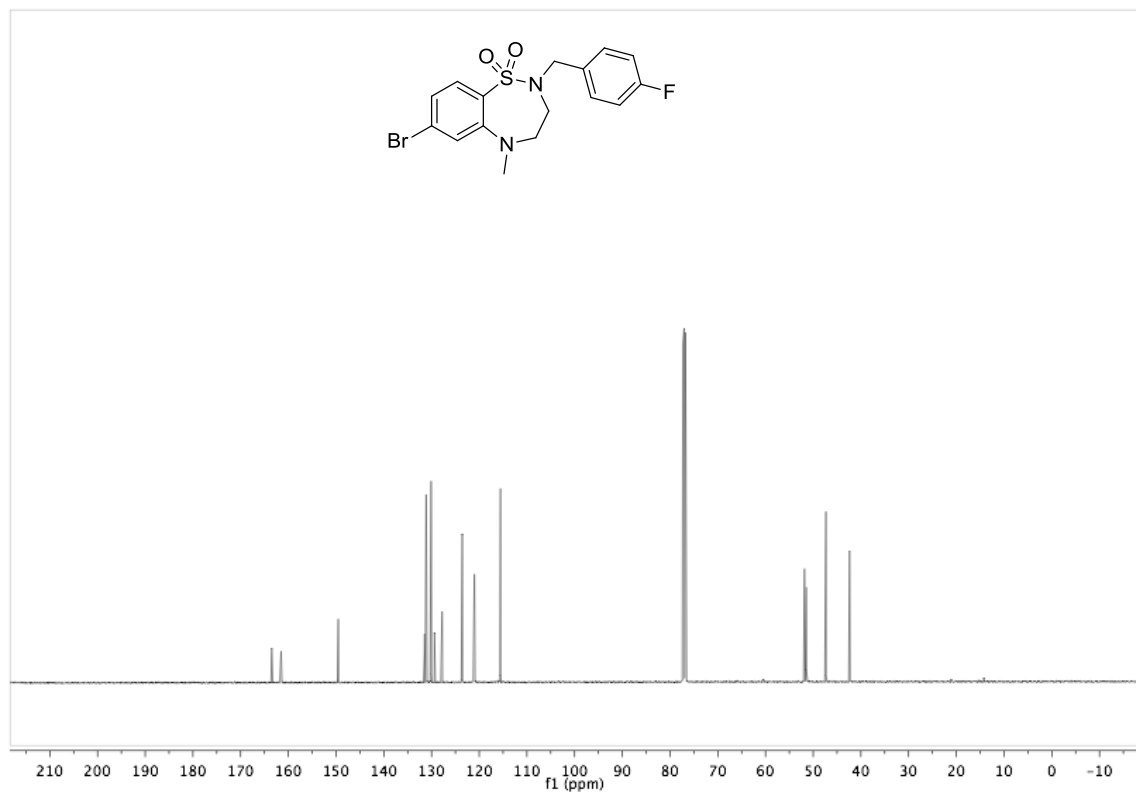
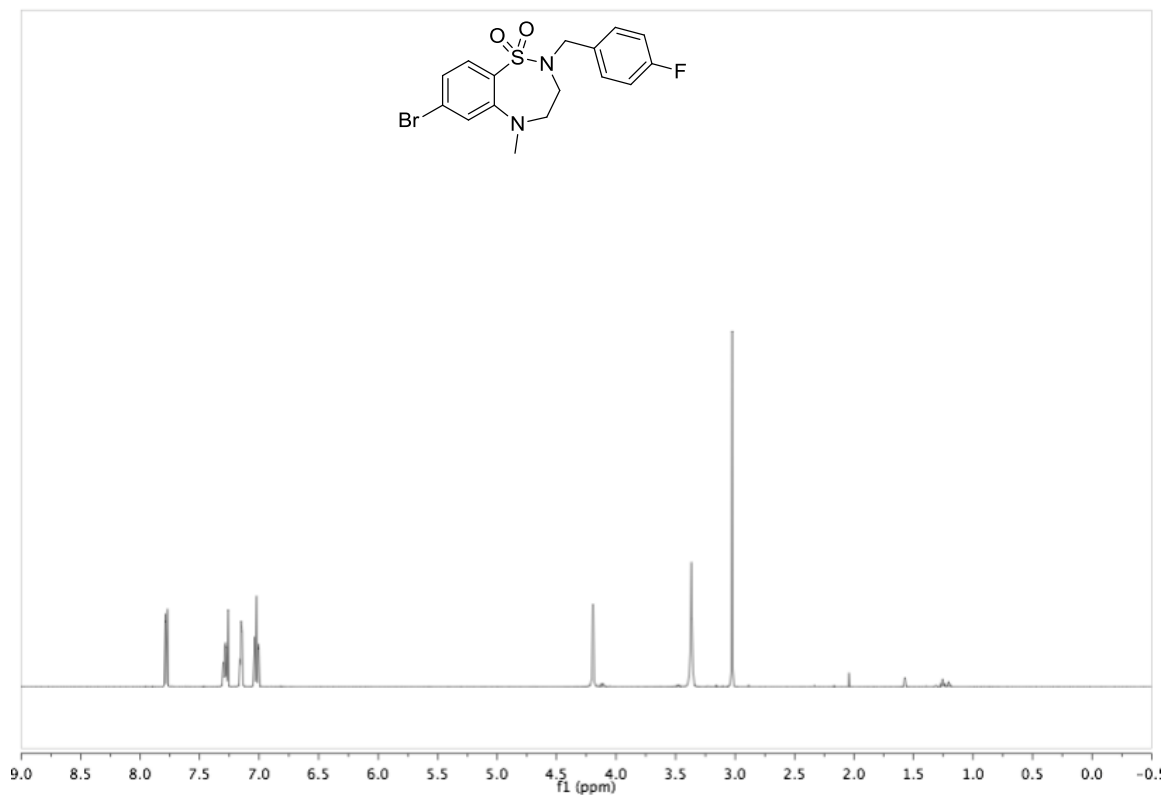
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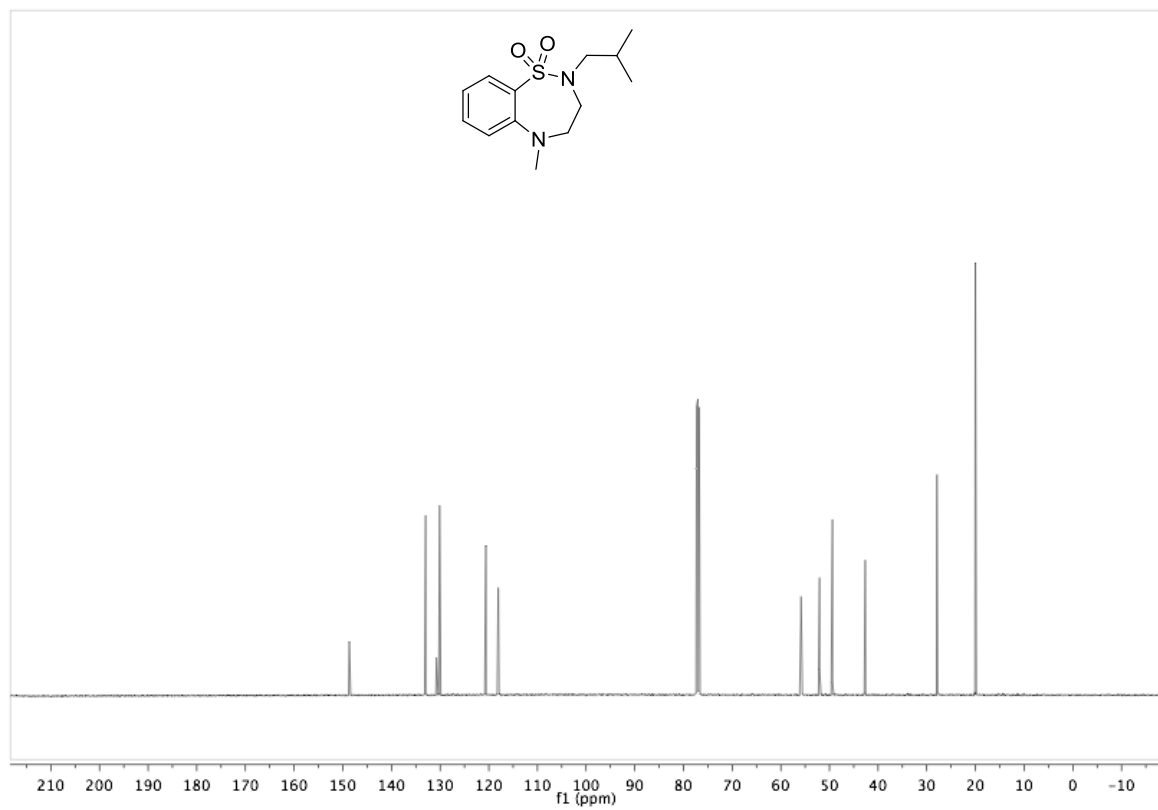
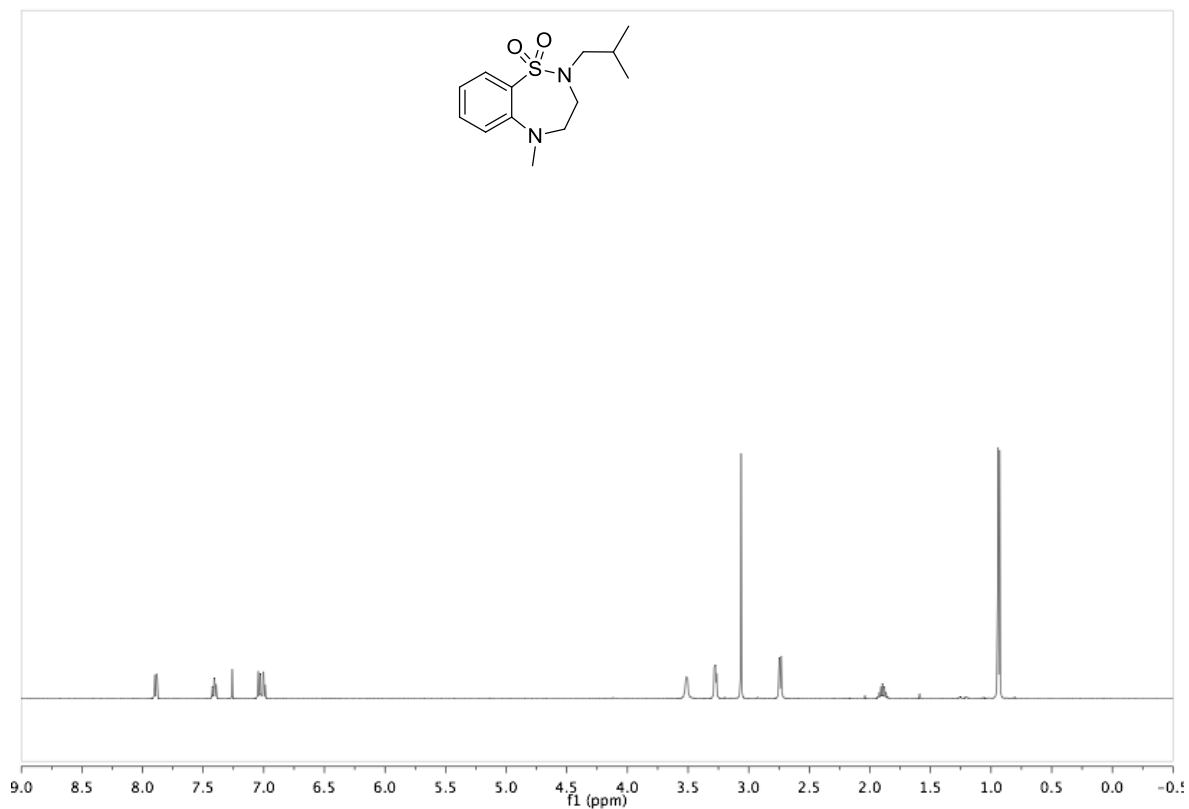
**(S)-2-bromo-6-(4-fluorobenzyl)-6,7,7a,8,9,10-hexahydrobenzo[f]pyrrolo[2,1-d][1,2,5] thiadiazepine 5,5-dioxide (3i)**



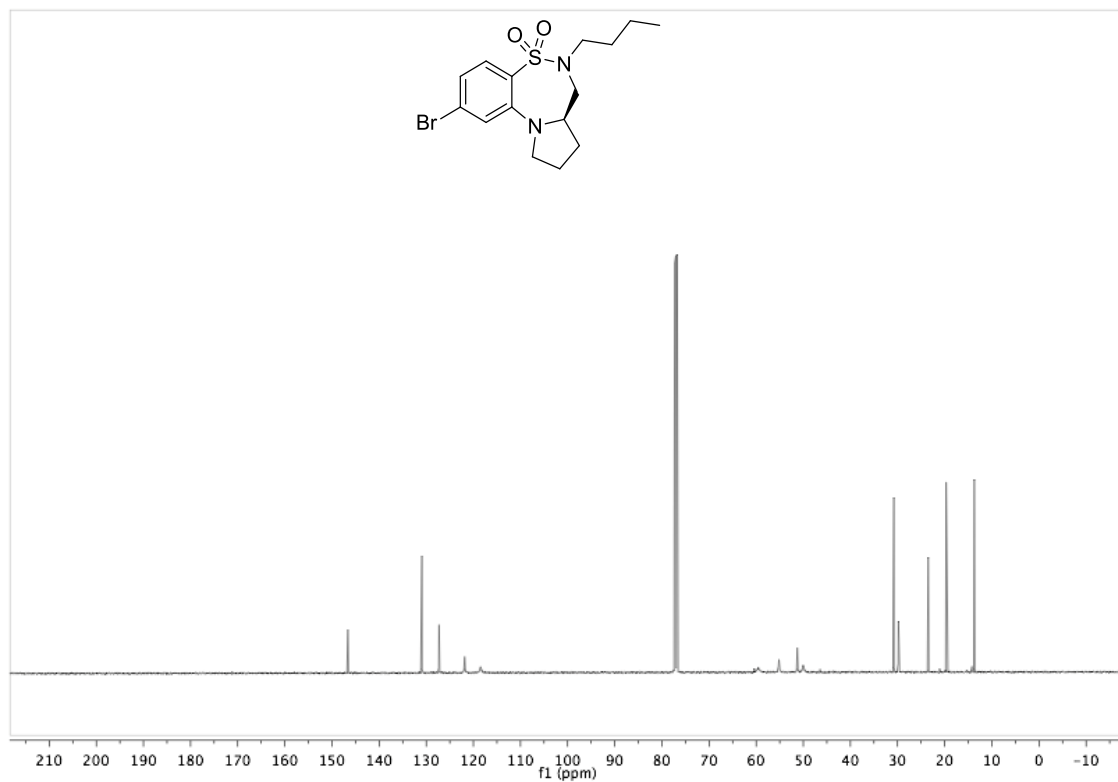
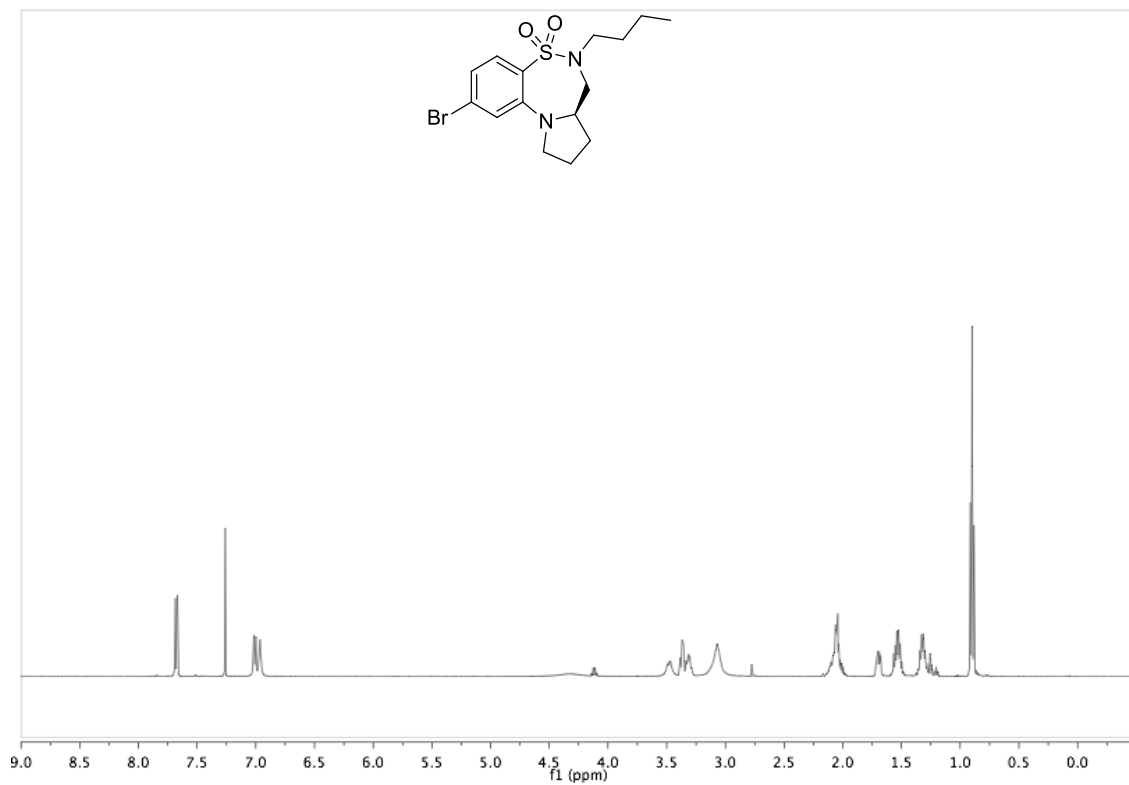


**2-Cyclopentyl-5-methyl-2,3,4,5-tetrahydrobenzo[*f*][1,2,5]thiadiazepine 1,1-dioxide (3j)**

**7-Bromo-2-(4-fluorobenzyl)-5-methyl-2,3,4,5-tetrahydrobenzo[f][1,2,5]thia-di-azepine 1,1-dioxide (3k)**

**2-Isobutyl-5-methyl-2,3,4,5-tetrahydrobenzo[f][1,2,5]thiadiazepine 1,1-di-oxide (3l)**

**(*R*)-2-Bromo-6-butyl-6,7,7a,8,9,10-hexahydrobenzo[*f*]pyrrolo[2,1-*d*][1,2,5] thiadiazepine 5,5-dioxide (3m)**



**8-Chloro-2-(4-chlorobenzyl)-5-methyl-2,3,4,5-tetrahydrobenzo[f][1,2,5]thia-diazepine 1,1-dioxide (3n)**